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Design of Anion–π Interactions and Hydrogen Bonds to Recognition of the Chloride, Bromide and Nitrate Anions

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Supplementary Material

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Table S1. Optimized Cartesian coordinates for the compounds investigated in this study using the B97D3/6–31+G(d) + PCM(DMSO) computational model.

Compound		**1**···Cl⁻	
Atom	X	Y	Z
C	–3.905271	–2.732627	–4.263589
C	–4.605072	–1.660825	–3.751756
C	–3.923185	–0.534436	–3.184528
C	–2.467833	–0.512987	–3.160203
C	–1.785953	–1.658839	–3.695796
C	–2.478399	–2.728444	–4.228001
C	–4.640277	0.544018	–2.643169
C	–3.988631	1.647274	–2.067968
C	–2.535546	1.686675	–2.043214
C	–1.795533	0.610131	–2.605393
C	–4.734763	2.732338	–1.501934
C	–4.096024	3.810217	–0.925633
C	–2.669987	3.853918	–0.893400
C	–1.916212	2.830244	–1.434461
C	–0.279260	0.638535	–2.555311
N	0.208736	0.115697	–1.264184
C	0.982064	0.803384	–0.430497
C	1.496128	0.530307	0.881110
C	2.211792	1.840014	0.917791
C	1.661154	2.122020	–0.470904
N	1.292524	–0.558526	1.648501
O	2.939184	2.461235	1.705181
O	1.735928	3.055844	–1.282910
C	1.784315	–0.866406	2.934083
C	1.380882	–2.097696	3.495592
C	1.832118	–2.468532	4.767411
C	2.687352	–1.623854	5.494327
C	3.084379	–0.401001	4.928976
C	2.642115	–0.013926	3.656469
H	–4.434459	–3.585915	–4.689832
H	–5.696701	–1.651517	–3.763261
H	–0.699156	–1.705758	–3.674138
H	–1.927974	–3.584441	–4.621072
H	–5.732174	0.520540	–2.662023
H	–5.824904	2.683218	–1.534850
H	–4.673737	4.628960	–0.494566
H	–2.168054	4.707776	–0.435675
H	–0.832671	2.905575	–1.390696
H	0.157418	0.042470	–3.364610
H	0.112399	1.652066	–2.672833
H	–0.153311	–0.801660	–0.954416
H	0.675119	–1.282461	1.235378
H	0.716615	–2.752895	2.930421
H	1.512439	–3.422510	5.189680
H	3.748445	0.265537	5.482143
H	2.954965	0.937414	3.228571
H	3.038345	–1.914141	6.485306
Cl	–0.664359	–2.672721	0.170622
Compound		**1**···Br⁻	
Atom	X	Y	Z
C	–3.708586	–2.860744	–4.020856
C	–4.425905	–1.842498	–3.429877
C	–3.774382	–0.653347	–2.964781
C	–2.337203	–0.508772	–3.133031
C	–1.635156	–1.599687	–3.749122
C	–2.295545	–2.734194	–4.176199
C	–4.504655	0.370393	–2.341036
C	–3.877410	1.524714	–1.843710

C	–2.441125	1.683450	–2.003843
C	–1.695993	0.670077	–2.665912
C	–4.630783	2.547572	–1.180185
C	–4.012141	3.670487	–0.671731
C	–2.600080	3.824671	–0.808761
C	–1.841589	2.866443	–1.453233
C	–0.185481	0.776067	–2.737611
N	0.380099	0.195721	–1.500997
C	1.103083	0.880805	–0.618609
C	1.509221	0.598691	0.726337
C	2.285472	1.871795	0.803901
C	1.834666	2.170342	–0.621729
N	1.166955	–0.454567	1.493952
O	2.987045	2.460762	1.636655
O	1.985076	3.101139	–1.425400
C	1.586328	–0.806113	2.792872
C	0.967724	–1.930837	3.381160
C	1.344157	–2.342691	4.664291
C	2.334817	–1.645107	5.375439
C	2.944409	–0.526620	4.783708
C	2.580835	–0.101631	3.498434
H	–4.213070	–3.764368	–4.365801
H	–5.506510	–1.925387	–3.298113
H	–0.555132	–1.553669	–3.872295
H	–1.728820	–3.548696	–4.629842
H	–5.583825	0.255388	–2.217141
H	–5.709557	2.412744	–1.079937
H	–4.594889	4.439957	–0.163564
H	–2.113191	4.710934	–0.398985
H	–0.768491	3.023667	–1.534994
H	0.218235	0.238936	–3.602829
H	0.161810	1.808254	–2.821857
H	–0.089401	–0.661297	–1.163576
H	0.461119	–1.092551	1.082808
H	0.197709	–2.469682	2.827189
H	0.859488	–3.213344	5.108913
H	3.715241	0.025164	5.324479
H	3.052557	0.772181	3.051793
H	2.626992	–1.968247	6.375296
Br	–1.249152	–2.303017	0.059071

Compound		**1**···NO_3^-	
Atom	X	Y	Z
C	–3.784067	–2.873554	–3.860130
C	–4.494744	–1.804094	–3.358100
C	–3.829180	–0.608890	–2.930700
C	–2.381992	–0.514056	–3.043051
C	–1.686763	–1.658106	–3.564075
C	–2.362626	–2.796165	–3.957975
C	–4.552240	0.468523	–2.395107
C	–3.912049	1.636518	–1.949907
C	–2.465616	1.746784	–2.056540
C	–1.723824	0.673631	–2.621242
C	–4.663279	2.717878	–1.383510
C	–4.035308	3.856351	–0.924037
C	–2.615413	3.966919	–1.014272
C	–1.857442	2.950374	–1.562780
C	–0.209676	0.747463	–2.685068
N	0.370415	0.182580	–1.450249
C	1.035211	0.894935	–0.544046
C	1.468149	0.588766	0.786172
C	2.118993	1.924779	0.927816
C	1.651191	2.242406	–0.488047

N	1.241654	–0.540861	1.484708
O	2.759936	2.539162	1.790470
O	1.733978	3.212348	–1.254395
C	1.652972	–0.901052	2.783182
C	1.184963	–2.133861	3.287470
C	1.563859	–2.556291	4.566723
C	2.407190	–1.759733	5.358801
C	2.867211	–0.533616	4.851087
C	2.500144	–0.097246	3.570888
H	–4.300537	–3.780500	–4.177194
H	–5.581838	–1.850250	–3.268867
H	–0.601444	–1.647246	–3.643596
H	–1.802362	–3.649239	–4.343384
H	–5.638554	0.391384	–2.310904
H	–5.748251	2.615333	–1.318776
H	–4.616540	4.671232	–0.490383
H	–2.121157	4.866524	–0.644205
H	–0.778526	3.077305	–1.608463
H	0.181217	0.191326	–3.544723
H	0.153290	1.772268	–2.786757
H	0.024663	–0.740643	–1.152342
H	0.642352	–1.232075	1.001258
H	0.529839	–2.754809	2.674659
H	1.195579	–3.511484	4.944029
H	3.522724	0.095684	5.455555
H	2.857588	0.857936	3.189001
H	2.701087	–2.089692	6.355855
N	–1.616550	–2.250713	0.197360
O	–2.047116	–1.185998	0.712123
O	–2.359813	–3.244057	0.007651
O	–0.368934	–2.323416	–0.146489

Compound		**2**···Cl^-	
Atom	X	Y	Z
C	–3.659884	–2.733283	–4.357258
C	–4.455875	–1.656335	–4.045509
C	–3.926192	–0.508154	–3.372597
C	–2.505613	–0.455922	–3.032634
C	–1.743250	–1.631854	–3.352230
C	–2.291575	–2.721167	–3.992703
C	–4.722292	0.595534	–3.028768
C	–4.246665	1.707490	–2.314960
C	–2.824297	1.746393	–1.981519
C	–1.958366	0.704131	–2.416839
C	–5.099937	2.789335	–1.924127
C	–4.615305	3.861425	–1.211984
C	–3.249162	3.895575	–0.842566
C	–2.394849	2.877713	–1.207644
C	–0.449300	0.851868	–2.284806
N	0.025389	0.326072	–0.996231
C	1.100202	0.785632	–0.365081
C	1.723404	0.429901	0.874692
C	2.782524	1.465687	0.686548
C	2.110006	1.839285	–0.628732
N	1.342948	–0.517180	1.755966
O	3.778756	1.873100	1.298982
O	2.317262	2.665162	–1.527714
C	1.928283	–0.904423	2.979113
C	1.281762	–1.930246	3.702686
C	1.809366	–2.364965	4.923886
C	2.981832	–1.787945	5.439373
C	3.619104	–0.768252	4.713645
C	3.104683	–0.320918	3.488944

H	–0.157819	1.899354	–2.361049
H	–0.496566	–0.459788	–0.572614
H	0.486086	–1.040478	1.499852
H	0.371169	–2.377860	3.301955
H	1.299740	–3.158369	5.472842
H	4.530863	–0.310638	5.101639
H	3.606323	0.471617	2.935561
H	3.391860	–2.127790	6.391137
Cl	–1.372722	–2.010850	0.732644
F	–1.126782	2.987471	–0.745711
F	–2.806349	4.927443	–0.099902
F	–5.420996	4.873112	–0.839105
F	–6.416789	2.792037	–2.226879
F	–6.022639	0.583923	–3.398017
F	–5.760903	–1.731480	–4.387582
F	–4.161710	–3.813686	–4.983795
F	–1.544612	–3.810581	–4.252467
F	–0.444603	–1.762797	–2.987919
H	0.047902	0.332943	–3.109548

Compound		**2**···Br⁻	
Atom	X	Y	Z
C	–3.458371	–2.915168	–3.890671
C	–4.291761	–1.904586	–3.474616
C	–3.771591	–0.651597	–3.015947
C	–2.328856	–0.421678	–2.994173
C	–1.519407	–1.527366	–3.431097
C	–2.057648	–2.719993	–3.860136
C	–4.607338	0.382092	–2.566743
C	–4.136432	1.589657	–2.028694
C	–2.690018	1.793646	–1.975457
C	–1.812323	0.821966	–2.531983
C	–5.021042	2.608354	–1.547147
C	–4.539736	3.762163	–0.975422
C	–3.142151	3.947474	–0.851138
C	–2.259329	2.998021	–1.317986
C	–0.308215	1.058803	–2.535333
N	0.229373	0.480194	–1.294295
C	1.245574	0.940634	–0.575549
C	1.738380	0.537745	0.705836
C	2.836004	1.546265	0.649269
C	2.296494	1.976917	–0.714279
N	1.227196	–0.407795	1.521382
O	3.779263	1.905945	1.365676
O	2.598369	2.826967	–1.561253
C	1.687005	–0.879798	2.767295
C	0.897804	–1.856080	3.413279
C	1.303560	–2.374502	4.648074
C	2.487169	–1.924408	5.256591
C	3.262811	–0.948295	4.609830
C	2.873994	–0.421805	3.370426
H	–0.064856	2.118128	–2.580023
H	–0.342557	–0.273869	–0.877255
H	0.358597	–0.860201	1.189021
H	–0.021312	–2.203318	2.938700
H	0.688438	–3.131587	5.136955
H	4.184114	–0.588727	5.071316
H	3.479412	0.338153	2.878137
H	2.800389	–2.329037	6.219729
Br	–1.678783	–1.738606	0.260288
F	–0.951112	3.267329	–1.085349
F	–2.690531	5.057620	–0.236917
F	–5.372247	4.715532	–0.516860

F	–6.363277	2.468639	–1.620728
F	–5.944943	0.198027	–2.641159
F	–5.621041	–2.148388	–3.504017
F	–3.947849	–4.096245	–4.312815
F	–1.256537	–3.738334	–4.228629
F	–0.164398	–1.493492	–3.397183
H	0.154127	0.591850	–3.407974
Compound		**2**···NO_3^-	
Atom	X	Y	Z
C	–3.559552	–2.872526	–4.312074
C	–4.368908	–1.834778	–3.913822
C	–3.829204	–0.669866	–3.278756
C	–2.386888	–0.555966	–3.071912
C	–1.608088	–1.694340	–3.476069
C	–2.165205	–2.801859	–4.076311
C	–4.638134	0.390842	–2.843156
C	–4.148574	1.511967	–2.153651
C	–2.704683	1.612525	–1.952317
C	–1.836737	0.621100	–2.490693
C	–5.011147	2.542614	–1.659000
C	–4.513053	3.620980	–0.966001
C	–3.121814	3.712579	–0.722419
C	–2.258980	2.746169	–1.192089
C	–0.326187	0.823306	–2.474779
N	0.244927	0.263010	–1.242041
C	1.230555	0.803043	–0.532575
C	1.762146	0.460102	0.749890
C	2.780320	1.548622	0.666167
C	2.196106	1.915120	–0.697332
N	1.330419	–0.508968	1.582403
O	3.700816	1.989892	1.365750
O	2.424038	2.773397	–1.559031
C	1.816443	–0.897778	2.846360
C	1.090862	–1.892669	3.536787
C	1.525548	–2.331325	4.792656
C	2.681137	–1.786211	5.376376
C	3.396630	–0.795446	4.684103
C	2.976997	–0.347239	3.424265
H	0.123685	0.349428	–3.351826
H	–0.074260	1.881898	–2.529511
H	–0.235211	–0.548660	–0.830642
H	0.484336	–1.009627	1.261944
H	0.192004	–2.316431	3.086195
H	0.956009	–3.101055	5.315626
H	4.295922	–0.362741	5.125823
H	3.534845	0.426402	2.898619
N	–2.105887	–1.296240	0.688356
O	–2.096818	–0.205282	1.315387
O	–3.174520	–1.890025	0.403945
O	–0.977941	–1.818339	0.317662
H	3.018372	–2.128423	6.355402
F	–0.960406	2.908729	–0.845096
F	–2.659636	4.747682	0.003501
F	–5.326662	4.584057	–0.494939
F	–6.349001	2.487862	–1.839721
F	–5.965317	0.323718	–3.089608
F	–5.695681	–1.965871	–4.132178
F	–4.070028	–3.969436	–4.901621
F	–1.398396	–3.854642	–4.416357
F	–0.276866	–1.773337	–3.230221
Compound		**3**···Cl^-	
Atom	X	Y	Z

C	–3.688642	–2.692810	–4.522299
C	–4.457566	–1.682819	–3.984344
C	–3.851647	–0.554348	–3.340457
C	–2.401115	–0.463589	–3.265618
C	–1.645271	–1.546341	–3.831936
C	–2.265686	–2.621034	–4.437913
C	–4.638070	0.460050	–2.772027
C	–4.060478	1.561981	–2.120368
C	–2.612432	1.669530	–2.042516
C	–1.803098	0.660736	–2.633606
C	–4.877586	2.579043	–1.526686
C	–4.312413	3.653971	–0.873310
C	–2.892149	3.762996	–0.786937
C	–2.071172	2.806867	–1.353030
C	–0.291957	0.751761	–2.531440
N	0.182250	0.130775	–1.278956
C	0.856904	0.779933	–0.335764
C	1.298066	0.421994	0.971993
C	1.898150	1.752596	1.212561
C	1.456827	2.142409	–0.199555
N	1.135903	–0.706309	1.693854
O	2.473695	2.310279	2.154871
O	1.523659	3.147733	–0.914693
C	1.741968	–0.929071	2.942210
C	0.967729	–1.325847	4.048157
C	1.544342	–1.582226	5.295089
C	2.925186	–1.428451	5.465267
C	3.719386	–1.038310	4.380531
C	3.131650	–0.810637	3.133079
H	0.057055	1.787051	–2.542022
H	–0.161011	–0.816755	–1.054062
H	0.510423	–1.445410	1.304979
F	–0.370761	–1.447190	3.911190
F	0.775119	–1.951745	6.340026
F	5.054132	–0.915922	4.536634
F	3.929680	–0.504135	2.089043
F	3.488939	–1.662808	6.666564
Cl	–0.697699	–2.716110	0.082774
H	–0.994833	2.930649	–1.264325
H	–2.448327	4.613392	–0.267063
H	–4.943787	4.420360	–0.421826
H	–5.962255	2.479625	–1.600832
H	–5.726385	0.385673	–2.829575
H	–5.547309	–1.726088	–4.033174
H	–4.160447	–3.548678	–5.006691
H	–1.660666	–3.428438	–4.852832
H	–0.558584	–1.540011	–3.776672
H	0.194692	0.252917	–3.377316

Compound		**3**···Br⁻	
Atom	X	Y	Z
C	–3.568029	–2.783202	–4.304634
C	–4.304893	–1.877738	–3.571389
C	–3.695695	–0.702621	–3.021421
C	–2.281787	–0.450757	–3.251083
C	–1.558007	–1.426570	–4.016877
C	–2.177334	–2.551060	–4.524807
C	–4.447337	0.209781	–2.264719
C	–3.862988	1.354761	–1.698809
C	–2.449098	1.617750	–1.913858
C	–1.681557	0.713181	–2.697789
C	–4.638726	2.265329	–0.909332
C	–4.062085	3.378377	–0.334290

C	–2.672221	3.635906	–0.528925
C	–1.894261	2.787651	–1.293213
C	–0.179796	0.898603	–2.805395
N	0.447315	0.218039	–1.649856
C	1.045014	0.862515	–0.648465
C	1.356584	0.491197	0.690926
C	2.006106	1.789921	0.977252
C	1.672400	2.204277	–0.461403
N	1.054830	–0.613957	1.401961
O	2.546441	2.313842	1.957920
O	1.808370	3.214979	–1.157775
C	1.487872	–0.839002	2.719666
C	0.557383	–1.072307	3.748274
C	0.964193	–1.306021	5.064703
C	2.328708	–1.313287	5.377712
C	3.275544	–1.082423	4.372593
C	2.852494	–0.871653	3.057441
H	0.121452	1.948248	–2.789365
H	0.048961	–0.707719	–1.420817
H	0.393994	–1.300262	0.978454
F	–0.763661	–1.037007	3.469204
F	0.051005	–1.513365	6.035690
F	4.590752	–1.103797	4.671848
F	3.783902	–0.703044	2.095388
F	2.729470	–1.537010	6.644500
Br	–0.916244	–2.582700	–0.336837
H	–0.840733	3.025410	–1.418152
H	–2.217970	4.515295	–0.069822
H	–4.661233	4.061833	0.268870
H	–5.700259	2.052540	–0.768380
H	–5.508363	0.013926	–2.094379
H	–5.369078	–2.041218	–3.390795
H	–4.040080	–3.677014	–4.714835
H	–1.594637	–3.275041	–5.096319
H	–0.492790	–1.298756	–4.197336
H	0.220482	0.471408	–3.730349

Compound		**3**···NO_3^-	
Atom	X	Y	Z
C	–3.585921	–2.854670	–4.112712
C	–4.356481	–1.827077	–3.611347
C	–3.753983	–0.628300	–3.107655
C	–2.307143	–0.485207	–3.138520
C	–1.548113	–1.586476	–3.662669
C	–2.164669	–2.729276	–4.132975
C	–4.538799	0.406315	–2.574523
C	–3.961233	1.576341	–2.055459
C	–2.515367	1.734384	–2.079321
C	–1.710982	0.704860	–2.638848
C	–4.776112	2.612817	–1.493141
C	–4.210658	3.752258	–0.960749
C	–2.792267	3.909063	–0.969564
C	–1.973724	2.936855	–1.511154
C	–0.198687	0.820949	–2.617848
N	0.336935	0.188124	–1.395339
C	0.918607	0.855178	–0.402158
C	1.288267	0.475964	0.918912
C	1.841401	1.813240	1.228026
C	1.471906	2.228224	–0.202052
N	1.095622	–0.682714	1.586045
O	2.348031	2.360690	2.213216
O	1.553274	3.252015	–0.887035
C	1.645040	–0.966988	2.845596

C	0.837579	–1.480327	3.877834
C	1.361024	–1.794137	5.134817
C	2.720600	–1.583958	5.392963
C	3.548158	–1.082202	4.381681
C	3.015800	–0.798162	3.121071
H	–4.055128	–3.764708	–4.488800
H	–5.444629	–1.910356	–3.581881
H	–0.461010	–1.538165	–3.686604
H	–1.557417	–3.548858	–4.519863
H	–5.624923	0.292990	–2.551278
H	–5.859096	2.474963	–1.490728
H	–4.840143	4.532579	–0.530925
H	–2.347689	4.808842	–0.541470
H	–0.898517	3.097549	–1.492018
H	0.250743	0.333143	–3.490476
H	0.140871	1.858396	–2.632491
H	–0.005751	–0.754642	–1.167537
H	0.452093	–1.369199	1.145506
N	–1.789399	–2.190113	0.123133
O	–2.227620	–1.120787	0.617855
O	–2.547543	–3.144807	–0.174663
O	–0.514524	–2.310325	–0.090598
F	3.853012	–0.389999	2.144021
F	–0.482783	–1.662942	3.656698
F	0.558123	–2.273946	6.106877
F	3.232180	–1.871743	6.606058
F	4.865201	–0.908274	4.617607

Compound		**4**···Cl^-	
Atom	X	Y	Z
C	–4.558477	3.559533	–0.216684
C	–5.052855	2.322230	–0.556808
C	–4.336088	1.121781	–0.245187
C	–3.068125	1.200170	0.477126
C	–2.591169	2.525744	0.760698
C	–3.305963	3.657859	0.437035
C	–4.811328	–0.151595	–0.595736
C	–4.102120	–1.340364	–0.358024
C	–2.837081	–1.246542	0.367571
C	–2.380256	0.011964	0.850256
C	–4.583399	–2.619158	–0.786981
C	–3.865928	–3.769088	–0.553247
C	–2.617884	–3.692200	0.110378
C	–2.124878	–2.480720	0.544580
C	–1.211735	0.087210	1.823771
N	0.070322	0.228036	1.118774
C	1.217091	–0.278756	1.556916
C	2.539366	–0.280651	1.028935
C	3.064504	–1.088962	2.151359
C	1.651931	–1.072124	2.746350
N	3.043940	0.231095	–0.114248
O	4.156654	–1.583199	2.454879
O	1.097100	–1.528698	3.749716
C	4.412691	0.240535	–0.431408
C	4.857771	–0.247919	–1.673829
C	6.208551	–0.226024	–2.031316
C	7.155772	0.277245	–1.131905
C	6.739785	0.772525	0.109557
C	5.382263	0.768648	0.442038
F	3.961712	–0.768271	–2.541128
F	6.606582	–0.710244	–3.225908
F	7.648515	1.283906	0.965962
F	5.002729	1.318415	1.614509

F	8.461865	0.292689	–1.463190
F	–0.894315	–2.519165	1.107834
F	–1.906080	–4.821877	0.281214
F	–4.317335	–4.968547	–0.964343
F	–5.753173	–2.744207	–1.451535
F	–6.015586	–0.238206	–1.203385
F	–6.235174	2.285980	–1.209655
F	–5.231325	4.686020	–0.516372
F	–2.809910	4.880801	0.701934
F	–1.371720	2.741067	1.311974
H	–1.170325	–0.809557	2.442207
H	–1.356503	0.928073	2.508979
H	0.082615	0.741283	0.222428
H	2.372669	0.634747	–0.801056
Cl	0.660353	1.494908	–1.803816

Compound		**4**···Br⁻	
Atom	X	Y	Z
C	–4.994943	3.499123	0.376916
C	–5.219946	2.315252	–0.284309
C	–4.320294	1.207638	–0.154876
C	–3.188945	1.293737	0.766590
C	–2.966279	2.587743	1.354906
C	–3.842555	3.637401	1.189334
C	–4.467581	0.026704	–0.896508
C	–3.585844	–1.063354	–0.810801
C	–2.535416	–1.013096	0.202304
C	–2.379804	0.150732	1.008818
C	–3.686586	–2.193121	–1.683591
C	–2.818646	–3.254529	–1.580543
C	–1.818796	–3.242149	–0.581152
C	–1.692339	–2.173671	0.278805
C	–1.297220	0.189805	2.075327
N	–0.006038	0.455986	1.408218
C	1.182974	0.128589	1.910881
C	2.452143	–0.058879	1.298377
C	3.108668	–0.376273	2.587955
C	1.738391	–0.179209	3.259861
N	2.815810	–0.043193	–0.002771
O	4.244823	–0.697012	2.949949
O	1.277719	–0.276292	4.399702
C	4.138840	–0.184025	–0.451122
C	4.474501	–1.163418	–1.403920
C	5.783972	–1.316849	–1.867292
C	6.794898	–0.478512	–1.382386
C	6.486909	0.506986	–0.437059
C	5.169067	0.660327	0.001706
F	3.517909	–2.002912	–1.857490
F	6.081012	–2.276382	–2.767638
F	7.456124	1.328600	0.015998
F	4.886428	1.657601	0.866454
F	8.060482	–0.621566	–1.822362
F	–0.678724	–2.277445	1.171808
F	–0.974581	–4.288362	–0.499040
F	–2.899046	–4.307731	–2.415701
F	–4.623607	–2.251478	–2.656212
F	–5.507280	–0.060429	–1.756661
F	–6.314145	2.243450	–1.074325
F	–5.837387	4.541706	0.250597
F	–3.595331	4.832656	1.758993
F	–1.855402	2.866972	2.080597
H	–1.252038	–0.766056	2.602503
H	–1.502081	0.953011	2.825175

H	–0.055583	0.520394	0.378098
H	2.057651	–0.039767	–0.714855
Br	0.074165	0.107687	–1.908039
Compound		**4**···NO_3^-	
Atom	X	Y	Z
C	–3.406444	–2.786850	–4.712644
C	–4.246110	–1.781692	–4.293723
C	–3.758557	–0.674398	–3.526900
C	–2.334308	–0.577221	–3.216469
C	–1.527207	–1.689095	–3.637603
C	–2.034727	–2.744392	–4.362586
C	–4.600838	0.343098	–3.053716
C	–4.161305	1.406605	–2.248390
C	–2.729467	1.509531	–1.974153
C	–1.825357	0.559863	–2.528439
C	–5.062890	2.379822	–1.709367
C	–4.613104	3.412071	–0.919798
C	–3.233101	3.514067	–0.623643
C	–2.334195	2.600208	–1.129017
C	–0.319023	0.769754	–2.429221
N	0.206822	0.170716	–1.192704
C	1.113501	0.728338	–0.396652
C	1.560631	0.391207	0.909848
C	2.515427	1.521309	0.954976
C	2.050800	1.888426	–0.463611
N	1.141100	–0.576200	1.756297
O	3.309491	1.982690	1.780955
O	2.304378	2.768759	–1.288864
C	1.768438	–0.880216	2.973974
C	1.014944	–1.000807	4.156648
C	1.609674	–1.326569	5.378372
C	2.993531	–1.525226	5.445902
C	3.766137	–1.417512	4.283648
C	3.153605	–1.117929	3.063740
H	0.176956	0.332873	–3.300119
H	–0.075518	1.831848	–2.432542
H	–0.284074	–0.650289	–0.819380
H	0.253728	–1.056097	1.509939
N	–2.269118	–1.170740	0.663682
O	–2.286436	–0.036321	1.204694
O	–3.318178	–1.732800	0.264211
O	–1.131647	–1.774753	0.498803
F	–1.050898	2.770606	–0.734182
F	–2.817166	4.506255	0.185612
F	–5.463740	4.320000	–0.406478
F	–6.392301	2.312949	–1.941940
F	–5.911113	0.289627	–3.380540
F	–5.552031	–1.888113	–4.622848
F	–3.868167	–3.829155	–5.428171
F	–1.245124	–3.775233	–4.717299
F	–0.222660	–1.796898	–3.281861
F	–0.318075	–0.782794	4.117329
F	0.860639	–1.424843	6.495999
F	3.577962	–1.827862	6.622004
F	5.096016	–1.638423	4.339651
F	3.913228	–1.095611	1.948066
Compound		**5**···Cl^-	
Atom	X	Y	Z
C	–3.740165	–2.652761	–4.413938
C	–4.500267	–1.520836	–4.162249
C	–3.960398	–0.405565	–3.430493
C	–2.574251	–0.447393	–2.965970

C	–1.866364	–1.679135	–3.181960
C	–2.425763	–2.734978	–3.895962
C	–4.726787	0.750580	–3.163625
C	–4.239603	1.826421	–2.383059
C	–2.831382	1.810933	–1.988794
C	–2.003075	0.710736	–2.353708
C	–5.075728	2.932969	–2.021030
C	–4.569568	4.021569	–1.344088
C	–3.199335	4.037757	–0.990744
C	–2.366614	2.958869	–1.244307
C	–0.489077	0.821161	–2.253674
N	0.035754	0.355519	–0.957452
C	1.114516	0.834545	–0.358441
C	1.791781	0.450735	0.845260
C	2.793879	1.539106	0.687161
C	2.087134	1.931948	–0.604876
N	1.493912	–0.578726	1.668967
O	3.783111	1.968146	1.300481
O	2.271109	2.781109	–1.485854
C	2.103763	–0.978748	2.875191
C	1.607423	–2.148355	3.491180
C	2.162789	–2.594814	4.695684
C	3.215236	–1.887630	5.300487
C	3.703826	–0.725618	4.681090
C	3.158046	–0.263059	3.475729
H	–0.168498	1.855323	–2.383330
H	–0.423143	–0.460590	–0.536185
H	0.726867	–1.190379	1.351695
H	0.790999	–2.699011	3.021343
H	1.769551	–3.500031	5.160994
H	4.521417	–0.166085	5.139070
H	3.549327	0.635260	3.000107
H	3.647005	–2.236764	6.239170
Cl	–0.901647	–2.496776	0.340011
O	–1.094637	2.999727	–0.735974
H	–1.034804	3.815807	–0.196665
O	–2.730972	5.096149	–0.203990
H	–2.363993	5.796483	–0.778990
O	–5.413981	5.055018	–1.020299
H	–4.917577	5.684630	–0.459479
O	–6.438474	2.877182	–2.310268
H	–6.833550	3.763062	–2.197933
O	–5.985885	0.795223	–3.726469
H	–6.476373	1.586496	–3.393273
O	–5.788860	–1.592011	–4.646062
H	–6.235475	–0.736156	–4.446719
O	–4.250659	–3.723321	–5.106369
H	–5.169600	–3.491347	–5.350525
O	–1.726739	–3.895555	–4.070217
H	–0.862982	–3.733231	–3.625255
O	–0.586587	–1.949028	–2.696387
H	–0.656294	–2.185298	–1.725776
H	–0.031214	0.222626	–3.048079

Compound		**5**···Br⁻	
Atom	X	Y	Z
C	–3.624903	–2.657632	–4.381723
C	–4.420275	–1.545960	–4.148682
C	–3.927262	–0.417865	–3.404150
C	–2.554721	–0.429669	–2.902522
C	–1.824750	–1.655030	–3.070143
C	–2.318581	–2.704566	–3.837798
C	–4.720708	0.726236	–3.167162

C	–4.270939	1.817292	–2.385038
C	–2.867292	1.839923	–1.975399
C	–2.012285	0.753640	–2.314894
C	–5.137847	2.905060	–2.040667
C	–4.664643	4.011759	–1.369024
C	–3.297575	4.066688	–1.006176
C	–2.434749	3.008022	–1.243604
C	–0.502473	0.903841	–2.216715
N	0.017974	0.477979	–0.907885
C	1.159704	0.868312	–0.367146
C	1.845396	0.446518	0.818672
C	2.934449	1.436473	0.601259
C	2.216178	1.866698	–0.674347
N	1.477523	–0.530467	1.676270
O	3.978205	1.786513	1.172837
O	2.432297	2.685383	–1.577261
C	2.101993	–0.993214	2.851221
C	1.497876	–2.086362	3.509875
C	2.062232	–2.590815	4.686548
C	3.226407	–2.015367	5.222714
C	3.819840	–0.926988	4.562312
C	3.268379	–0.409374	3.382106
H	–0.207776	1.942755	–2.373861
H	–0.515245	–0.256478	–0.425532
H	0.626377	–1.051034	1.413642
H	0.594125	–2.532872	3.092354
H	1.587601	–3.436983	5.185870
H	4.724403	–0.470085	4.967526
H	3.737369	0.432214	2.873590
H	3.664019	–2.409444	6.140678
Br	–1.341630	–2.168046	0.584831
O	–1.165994	3.088666	–0.729444
H	–1.135169	3.908959	–0.193746
O	–2.862388	5.143874	–0.226043
H	–2.510581	5.848672	–0.805021
O	–5.537536	5.026483	–1.061667
H	–5.061677	5.675294	–0.504939
O	–6.495628	2.812097	–2.343400
H	–6.912246	3.690187	–2.248745
O	–5.967291	0.742704	–3.759065
H	–6.481878	1.523200	–3.437151
O	–5.696531	–1.650203	–4.658709
H	–6.166475	–0.803517	–4.474898
O	–4.088757	–3.737061	–5.093138
H	–5.006399	–3.527329	–5.361080
O	–1.584570	–3.844868	–4.003294
H	–0.743054	–3.670603	–3.522250
O	–0.552602	–1.894524	–2.547535
H	–0.664546	–2.073826	–1.571683
H	–0.028247	0.296628	–2.995616

Compound		**5**···NO_3^-	
Atom	X	Y	Z
C	–3.320715	–2.511136	–5.062001
C	–4.200708	–1.491305	–4.726952
C	–3.823314	–0.464745	–3.796622
C	–2.475352	–0.466886	–3.233531
C	–1.637874	–1.585225	–3.556017
C	–2.046656	–2.571507	–4.449383
C	–4.708720	0.571280	–3.415911
C	–4.384522	1.525905	–2.422017
C	–3.020372	1.539015	–1.899495
C	–2.063222	0.614242	–2.397002

C	–5.338115	2.479819	–1.936501
C	–4.995459	3.407744	–0.975983
C	–3.680761	3.415564	–0.448002
C	–2.731853	2.495296	–0.857617
C	–0.584491	0.862075	–2.176533
N	–0.058468	0.077401	–1.021720
C	1.251761	0.130657	–0.694283
C	1.955877	–0.157233	0.512528
C	3.274441	0.112497	–0.156543
C	2.493938	0.410808	–1.440877
N	1.455082	–0.487785	1.714827
O	4.466214	0.107768	0.156644
O	2.787718	0.746115	–2.593952
C	2.120710	–0.798593	2.919338
C	1.314519	–1.015101	4.057606
C	1.906819	–1.341325	5.282934
C	3.302704	–1.453266	5.391403
C	4.098246	–1.235265	4.254787
C	3.520811	–0.911526	3.019473
H	–0.014304	0.563614	–3.061962
H	–0.394360	1.924713	–2.006985
H	–0.707876	0.004777	–0.227254
H	0.418330	–0.483477	1.772033
H	0.231070	–0.923592	3.976232
H	1.272480	–1.506219	6.155117
H	5.184075	–1.319391	4.324150
H	4.148304	–0.739672	2.146832
N	–1.988667	0.469907	2.098697
O	–1.283878	1.353586	2.657316
O	–3.241840	0.532449	2.092088
O	–1.404620	–0.525027	1.515587
H	3.763069	–1.707183	6.346871
O	–0.385408	–1.834204	–3.015321
H	–0.295412	–1.414898	–2.122719
O	–1.245273	–3.648772	–4.719975
H	–0.448156	–3.542417	–4.158489
O	–3.678238	–3.507015	–5.937304
H	–4.593458	–3.315626	–6.226208
O	–5.437579	–1.592375	–5.331170
H	–5.976372	–0.818273	–5.047878
O	–5.922555	0.604439	–4.070077
H	–6.514219	1.277379	–3.657426
O	–6.640601	2.441705	–2.421329
H	–7.170720	3.143399	–1.996893
O	–5.951662	4.292263	–0.539191
H	–5.566661	4.804730	0.200665
O	–3.426788	4.262242	0.633417
H	–2.907801	5.034148	0.333321
O	–1.522228	2.460431	–0.206978
H	–1.625425	2.939405	0.641201

Compound		**6**···Cl^-	
Atom	X	Y	Z
C	–3.588978	–2.788946	–4.341411
C	–4.381807	–1.810218	–3.780844
C	–3.804007	–0.642345	–3.183270
C	–2.358258	–0.477184	–3.181320
C	–1.575992	–1.529162	–3.769078
C	–2.169213	–2.643822	–4.328317
C	–4.612611	0.339783	–2.589799
C	–4.061562	1.478553	–1.979893
C	–2.618853	1.660017	–1.973474
C	–1.789586	0.685364	–2.593142

C	–4.900152	2.460812	–1.358377
C	–4.359658	3.570763	–0.743909
C	–2.944194	3.751521	–0.726537
C	–2.103236	2.830903	–1.321482
C	–0.282623	0.852684	–2.565179
N	0.276562	0.262024	–1.331366
C	0.978112	0.940397	–0.433710
C	1.524710	0.588887	0.847979
C	2.124880	1.924006	1.003405
C	1.516355	2.325947	–0.321791
N	1.454478	–0.567119	1.526863
O	2.869478	2.471896	1.848682
O	1.475990	3.349495	–1.016762
C	1.772360	–0.825503	2.889301
C	0.837806	–1.571567	3.657225
C	1.136917	–1.885163	4.997479
C	2.342386	–1.456811	5.573973
C	3.257582	–0.718369	4.817260
C	2.986530	–0.406651	3.477075
H	–4.039064	–3.675615	–4.789688
H	–5.468970	–1.909246	–3.775370
H	–0.489608	–1.466844	–3.768606
H	–1.544403	–3.426317	–4.761262
H	–5.697086	0.209640	–2.592788
H	–5.980620	2.305946	–1.379100
H	–5.006800	4.310250	–0.270425
H	–2.519887	4.629124	–0.236379
H	–1.031331	3.009561	–1.284306
H	0.190158	0.371079	–3.428545
H	0.016137	1.903130	–2.593805
H	–0.019970	–0.695007	–1.089598
H	0.929975	–1.313195	1.039859
Cl	–0.496107	–2.636495	0.099528
O	–0.394277	–1.972009	3.197678
H	–0.411423	–2.113212	2.215317
O	0.222219	–2.604528	5.736052
H	0.592232	–2.719531	6.632880
O	2.563118	–1.790792	6.894637
H	3.436701	–1.447865	7.163105
O	4.430516	–0.317844	5.419593
H	4.926241	0.182980	4.736644
O	3.984535	0.267661	2.801363
H	3.636854	1.168412	2.512993

Compound		**6**···Br⁻	
Atom	X	Y	Z
C	–3.447456	–2.847748	–4.180116
C	–4.134816	–2.050899	–3.289749
C	–3.543854	–0.860051	–2.754530
C	–2.205985	–0.470824	–3.171805
C	–1.529843	–1.338309	–4.094720
C	–2.126939	–2.484381	–4.580584
C	–4.227264	–0.081827	–1.808212
C	–3.647017	1.063865	–1.239359
C	–2.316558	1.474219	–1.656337
C	–1.618017	0.701990	–2.625019
C	–4.342270	1.825090	–0.244146
C	–3.763775	2.934467	0.336402
C	–2.456833	3.341937	–0.064756
C	–1.759661	2.638795	–1.028538
C	–0.158262	1.007691	–2.904135
N	0.629313	0.342618	–1.836022
C	1.270369	1.002825	–0.875121

C	1.662423	0.628472	0.451173
C	2.345670	1.915286	0.662213
C	1.869751	2.357892	–0.710903
N	1.408301	–0.490924	1.148487
O	3.052797	2.404175	1.570882
O	1.924761	3.388659	–1.391503
C	1.489048	–0.675174	2.558750
C	0.348007	–1.188456	3.231433
C	0.415805	–1.419199	4.619530
C	1.588466	–1.127271	5.332943
C	2.701595	–0.601474	4.668876
C	2.661101	–0.375923	3.285585
H	–3.903286	–3.756733	–4.574995
H	–5.141688	–2.319322	–2.964013
H	–0.516283	–1.109871	–4.417544
H	–1.579643	–3.123954	–5.274669
H	–5.222151	–0.392630	–1.481285
H	–5.342217	1.500304	0.050107
H	–4.299251	3.502203	1.098484
H	–2.002048	4.221201	0.394046
H	–0.770366	2.991499	–1.309331
H	0.168587	0.630478	–3.877228
H	0.069241	2.075972	–2.885552
H	0.267835	–0.588596	–1.573976
H	0.847792	–1.193959	0.640110
Br	–0.771105	–2.425307	–0.464999
O	–0.875169	–1.403489	2.642677
H	–0.807746	–1.659930	1.684781
O	–0.694943	–1.910436	5.271026
H	–0.469080	–1.993211	6.217928
O	1.575893	–1.367620	6.691862
H	2.447478	–1.129216	7.061061
O	3.828510	–0.315240	5.408396
H	4.482006	0.051569	4.775190
O	3.820212	0.111003	2.710473
H	3.631122	1.029239	2.346086

Compound		**6**···NO_3^-	
Atom	X	Y	Z
C	–3.522754	–2.733493	–4.677929
C	–4.327369	–1.802821	–4.056020
C	–3.763578	–0.679916	–3.366591
C	–2.319155	–0.504672	–3.339003
C	–1.524199	–1.507125	–3.992649
C	–2.104192	–2.582037	–4.637119
C	–4.585438	0.242388	–2.700915
C	–4.049552	1.331776	–1.994979
C	–2.609999	1.530220	–1.972284
C	–1.766548	0.615839	–2.661249
C	–4.900413	2.247158	–1.293600
C	–4.374120	3.309473	–0.589000
C	–2.961684	3.510165	–0.561170
C	–2.109925	2.653332	–1.231260
C	–0.262510	0.800819	–2.602854
N	0.273068	0.206603	–1.359880
C	0.924900	0.887957	–0.426719
C	1.390181	0.551171	0.889996
C	2.056103	1.858925	1.028804
C	1.507196	2.255036	–0.324175
N	1.217996	–0.561720	1.620287
O	2.819735	2.381883	1.871718
O	1.527449	3.263577	–1.041645
C	1.614116	–0.797017	2.966859

C	0.677345	–1.414544	3.835222
C	1.069216	–1.769437	5.141428
C	2.364974	–1.483087	5.593728
C	3.275344	–0.837067	4.749797
C	2.911348	–0.495452	3.440771
H	0.236232	0.333860	–3.458555
H	0.022997	1.855811	–2.613891
H	–0.027041	–0.746941	–1.128185
H	0.622473	–1.280466	1.175705
N	–1.807795	–1.866966	0.343990
O	–2.001965	–1.000653	1.257571
O	–2.762065	–2.377744	–0.273088
O	–0.596905	–2.201678	0.057959
H	–0.438163	–1.439462	–3.976420
H	–1.469521	–3.327716	–5.118132
H	–3.962255	–3.587579	–5.194777
H	–5.413842	–1.908789	–4.068279
H	–5.668298	0.100239	–2.718768
H	–5.978678	2.079671	–1.326631
H	–5.030372	3.997377	–0.054294
H	–2.548515	4.352256	–0.003866
H	–1.041334	2.847390	–1.187519
O	3.900763	0.083541	2.668393
H	3.609357	1.016169	2.435121
O	–0.605045	–1.734667	3.479794
H	–0.904431	–1.300604	2.637870
O	0.152483	–2.383791	5.967591
H	0.584920	–2.531570	6.830899
O	2.674287	–1.840448	6.889950
H	3.594578	–1.574295	7.077157
O	4.531228	–0.551963	5.242025
H	5.011030	–0.102090	4.514096

Compound		**7**···Cl^-	
Atom	X	Y	Z
C	–3.504541	–2.635370	–4.580254
C	–4.334191	–1.564342	–4.284376
C	–3.867173	–0.450352	–3.502082
C	–2.483988	–0.429007	–3.029015
C	–1.703419	–1.605236	–3.290051
C	–2.189775	–2.660312	–4.056221
C	–4.702226	0.647134	–3.195886
C	–4.286876	1.710932	–2.358918
C	–2.885203	1.757278	–1.947054
C	–1.986543	0.733264	–2.363177
C	–5.188215	2.749702	–1.955894
C	–4.753104	3.827695	–1.214831
C	–3.392360	3.898426	–0.832108
C	–2.497862	2.882172	–1.129332
C	–0.482089	0.946776	–2.273854
N	0.100696	0.432139	–1.021879
C	1.094169	0.975795	–0.344439
C	1.768351	0.544165	0.848185
C	2.638065	1.724332	0.843676
C	1.944240	2.203419	–0.416162
N	1.588157	–0.584099	1.561741
O	3.589785	2.135615	1.551306
O	2.058843	3.166810	–1.180632
C	1.996123	–0.884563	2.890556
C	1.034111	–1.468043	3.757994
C	1.399603	–1.810235	5.073362
C	2.704835	–1.567799	5.529075
C	3.649764	–0.992222	4.674386

C	3.310940	–0.658324	3.354031
H	–0.235829	2.007494	–2.336493
H	–0.297738	–0.438159	–0.653250
H	0.929434	–1.251724	1.137294
Cl	–0.734865	–2.486201	0.290790
O	–1.240186	2.952891	–0.590572
H	–1.226781	3.739205	–0.006138
O	–2.997759	4.932220	0.023665
H	–2.656113	5.682220	–0.502132
O	–5.659169	4.795290	–0.856454
H	–5.210310	5.421797	–0.253638
O	–6.540114	2.635517	–2.273985
H	–6.988652	3.487034	–2.108607
O	–5.953660	0.646050	–3.775252
H	–6.493654	1.391430	–3.414374
O	–5.614017	–1.693803	–4.776842
H	–6.111730	–0.873819	–4.549852
O	–3.944419	–3.703918	–5.321840
H	–4.874233	–3.518487	–5.564535
O	–1.422335	–3.767736	–4.277249
H	–0.567838	–3.577225	–3.827283
O	–0.413095	–1.815957	–2.795176
H	–0.481385	–2.122017	–1.851514
O	4.340790	–0.171677	2.576282
H	4.118822	0.759257	2.250441
O	4.922449	–0.777855	5.157307
H	5.424601	–0.371429	4.418448
O	2.991880	–1.916905	6.833054
H	3.930810	–1.718433	7.011370
O	0.455924	–2.369795	5.907502
H	0.884785	–2.534757	6.769657
O	–0.284358	–1.675832	3.416265
H	–0.400795	–1.837930	2.450357
H	0.004134	0.435572	–3.111623

Compound		**7**···Br⁻	
Atom	X	Y	Z
C	–3.417761	–2.599887	–4.654071
C	–4.276748	–1.565550	–4.314130
C	–3.835785	–0.466355	–3.497008
C	–2.452939	–0.427978	–3.026767
C	–1.651747	–1.584844	–3.307337
C	–2.096654	–2.602661	–4.144389
C	–4.692262	0.604221	–3.157682
C	–4.293741	1.654586	–2.295746
C	–2.887171	1.729433	–1.905211
C	–1.971388	0.738068	–2.358029
C	–5.216084	2.656525	–1.850562
C	–4.797327	3.725132	–1.086857
C	–3.432468	3.823633	–0.724580
C	–2.515041	2.841385	–1.063295
C	–0.472555	0.989924	–2.294289
N	0.123993	0.473319	–1.052670
C	1.178276	0.948044	–0.420297
C	1.840624	0.487146	0.766561
C	2.818543	1.576096	0.708809
C	2.125502	2.098306	–0.537658
N	1.573620	–0.596547	1.521144
O	3.827911	1.903374	1.379064
O	2.284462	3.043565	–1.316835
C	1.959129	–0.864639	2.863607
C	0.943925	–1.257275	3.775745
C	1.287895	–1.563172	5.105589

C	2.621864	–1.462475	5.531608
C	3.616867	–1.062131	4.634536
C	3.298231	–0.769812	3.299413
H	–0.255899	2.058011	–2.352849
H	–0.349413	–0.335896	–0.632042
H	0.843058	–1.212076	1.138303
Br	–1.089884	–2.322581	0.321967
O	–1.249109	2.934985	–0.544884
H	–1.253365	3.698824	0.068940
O	–3.053369	4.844229	0.153866
H	–2.741938	5.617986	–0.356176
O	–5.723023	4.657100	–0.686191
H	–5.282774	5.273787	–0.067109
O	–6.568844	2.513349	–2.151313
H	–7.039854	3.343447	–1.944748
O	–5.947500	0.590803	–3.729448
H	–6.503505	1.309047	–3.339687
O	–5.557770	–1.715793	–4.797899
H	–6.074280	–0.915754	–4.543740
O	–3.829839	–3.650022	–5.436979
H	–4.765801	–3.482412	–5.668668
O	–1.296668	–3.674880	–4.418385
H	–0.450814	–3.484181	–3.952337
O	–0.351816	–1.776428	–2.830317
H	–0.424921	–2.063325	–1.882133
O	4.361659	–0.444850	2.482320
H	4.236548	0.488196	2.115882
O	4.912957	–0.973855	5.093400
H	5.449204	–0.671853	4.328994
O	2.885270	–1.764232	6.852216
H	3.844456	–1.674096	7.009443
O	0.297194	–1.940004	5.986266
H	0.718341	–2.101149	6.853000
O	–0.399970	–1.285345	3.471104
H	–0.568711	–1.519867	2.527692
H	0.013921	0.497473	–3.143378

Compound		**7**···NO_3^-	
Atom	X	Y	Z
C	–2.868345	–2.522535	–5.163764
C	–3.860414	–1.591057	–4.891554
C	–3.644104	–0.534947	–3.942269
C	–2.343344	–0.410710	–3.288156
C	–1.381908	–1.440337	–3.558416
C	–1.636340	–2.460022	–4.471142
C	–4.646925	0.413595	–3.630854
C	–4.482642	1.400179	–2.628883
C	–3.169268	1.534127	–2.003942
C	–2.098903	0.697171	–2.420949
C	–5.550452	2.269119	–2.228760
C	–5.365748	3.226454	–1.254001
C	–4.101538	3.351353	–0.627712
C	–3.047082	2.516332	–0.953161
C	–0.673048	1.067256	–2.069103
N	–0.190708	0.313104	–0.875420
C	1.053578	0.479425	–0.395866
C	1.683863	0.101501	0.832400
C	3.004467	0.541763	0.323416
C	2.323782	0.998797	–0.958610
N	1.179075	–0.435738	1.952027
O	4.178574	0.470831	0.733638
O	2.678270	1.539279	–2.011087
C	1.865208	–0.757853	3.157387

C	1.245533	–0.425279	4.389440
C	1.847972	–0.826168	5.599640
C	3.063595	–1.523458	5.590597
C	3.689821	–1.824223	4.375610
C	3.097913	–1.451078	3.162712
H	–0.002665	0.829385	–2.900687
H	–0.588340	2.138000	–1.873915
H	–0.910126	0.072867	–0.182686
H	0.153372	–0.575487	1.939422
N	–2.255717	0.497542	2.008490
O	–1.560613	1.356154	2.641936
O	–3.481162	0.655807	1.847367
O	–1.667742	–0.539606	1.523779
O	3.761729	–1.850589	2.016009
H	4.086970	–1.029671	1.547889
O	0.063459	0.251556	4.507010
H	–0.290398	0.608507	3.650749
O	1.227264	–0.505546	6.787603
H	1.787078	–0.841385	7.514225
O	3.602512	–1.867991	6.812466
H	4.441653	–2.343596	6.662456
O	4.892877	–2.495778	4.412247
H	5.166705	–2.614253	3.477806
O	–1.896369	2.591938	–0.207236
H	–2.104824	3.106898	0.599398
O	–4.000607	4.216730	0.464698
H	–3.587527	5.056879	0.183873
O	–6.427678	4.023412	–0.900854
H	–6.159599	4.548663	–0.119670
O	–6.802562	2.118868	–2.813758
H	–7.430724	2.750490	–2.413603
O	–5.812236	0.327053	–4.362577
H	–6.490727	0.944718	–3.999816
O	–5.037763	–1.806596	–5.577825
H	–5.666639	–1.089300	–5.332771
O	–3.070944	–3.545826	–6.056445
H	–3.979906	–3.442725	–6.404311
O	–0.718118	–3.451696	–4.688441
H	0.027042	–3.269914	–4.076770
O	–0.137488	–1.562275	–2.954074
H	–0.153023	–1.192062	–2.039207

Compound		**1**	
Atom	X	Y	Z
C	–3.872315	–2.776830	–4.108103
C	–4.584548	–1.688172	–3.651451
C	–3.915862	–0.529097	–3.137514
C	–2.461559	–0.492229	–3.109915
C	–1.765512	–1.653984	–3.590416
C	–2.445776	–2.755898	–4.071058
C	–4.643750	0.568562	–2.651630
C	–4.004187	1.703276	–2.126479
C	–2.551072	1.756431	–2.093851
C	–1.801319	0.661627	–2.605063
C	–4.763535	2.806946	–1.616821
C	–4.138090	3.915109	–1.085607
C	–2.712812	3.970831	–1.042418
C	–1.945885	2.930521	–1.530564
C	–0.286469	0.692981	–2.556423
N	0.209186	0.124751	–1.281957
C	0.954458	0.796045	–0.405168
C	1.470360	0.500827	0.895670
C	2.143768	1.832549	0.979429

C	1.590520	2.137318	–0.406991
N	1.314621	–0.615520	1.640554
O	2.844623	2.450117	1.786901
O	1.641249	3.090280	–1.192187
C	1.811255	–0.938902	2.925852
C	1.475306	–2.206700	3.444502
C	1.933856	–2.588453	4.710488
C	2.729142	–1.715988	5.470801
C	3.058812	–0.456153	4.946093
C	2.607809	–0.057939	3.680156
H	–4.391553	–3.654851	–4.494168
H	–5.676062	–1.690052	–3.667670
H	–0.677421	–1.683646	–3.576171
H	–1.885619	–3.622009	–4.426165
H	–5.735245	0.535411	–2.674474
H	–5.852823	2.747234	–1.656276
H	–4.725524	4.748298	–0.697742
H	–2.221471	4.847820	–0.618312
H	–0.863351	3.016774	–1.477551
H	0.152333	0.124876	–3.384533
H	0.109487	1.707593	–2.632396
H	–0.141193	–0.799670	–1.041126
H	0.749473	–1.352550	1.224430
H	0.857394	–2.889817	2.858598
H	1.666688	–3.571569	5.100188
H	3.675960	0.232233	5.525595
H	2.869868	0.921538	3.283962
H	3.086111	–2.013909	6.457098

Compound		**2**	
Atom	X	Y	Z
C	–3.727452	–2.700503	–4.425414
C	–4.495717	–1.587089	–4.176507
C	–3.968861	–0.461491	–3.463943
C	–2.577719	–0.472582	–3.018512
C	–1.852569	–1.687309	–3.265070
C	–2.394957	–2.753693	–3.947116
C	–4.735882	0.679891	–3.182291
C	–4.261543	1.772188	–2.436937
C	–2.864173	1.752194	–2.010204
C	–2.017697	0.668918	–2.379591
C	–5.089861	2.892976	–2.107582
C	–4.604113	3.951180	–1.375010
C	–3.263363	3.930809	–0.920802
C	–2.434394	2.871705	–1.221999
C	–0.508609	0.772120	–2.204419
N	–0.055540	0.271473	–0.893292
C	1.009358	0.757919	–0.253971
C	1.676043	0.412048	0.960368
C	2.672334	1.512033	0.778688
C	1.948447	1.877618	–0.514720
N	1.390376	–0.577432	1.835075
O	3.656346	1.955953	1.376498
O	2.088846	2.729238	–1.396919
C	2.028261	–0.950634	3.041840
C	1.504867	–2.067611	3.725543
C	2.086215	–2.487218	4.927431
C	3.191166	–1.802784	5.458999
C	3.706104	–0.692777	4.770548
C	3.135030	–0.258313	3.566456
H	–0.182646	1.808474	–2.291508
H	–0.490797	–0.584653	–0.560871
H	0.584404	–1.154641	1.604591

H	0.647383	–2.605156	3.315884
H	1.671962	–3.352346	5.446734
H	4.564341	–0.151447	5.171725
H	3.543705	0.602938	3.040909
H	3.643655	–2.130191	6.395494
F	–1.195076	2.924195	–0.680205
F	–2.822968	4.949389	–0.159891
F	–5.387016	4.999063	–1.060194
F	–6.384044	2.947016	–2.490141
F	–6.003130	0.727223	–3.647188
F	–5.771241	–1.602810	–4.619428
F	–4.226842	–3.758123	–5.090351
F	–1.685560	–3.881603	–4.133165
F	–0.604366	–1.878698	–2.766505
H	–0.005571	0.220638	–3.004708

Compound		**3**	
Atom	X	Y	Z
C	–3.671550	–2.671540	–4.560672
C	–4.451694	–1.655578	–4.050612
C	–3.860257	–0.526589	–3.394677
C	–2.412464	–0.441576	–3.277219
C	–1.644050	–1.528602	–3.818525
C	–2.251363	–2.604192	–4.436867
C	–4.657972	0.495180	–2.855735
C	–4.095338	1.598108	–2.192917
C	–2.649720	1.699139	–2.069606
C	–1.828991	0.683164	–2.631819
C	–4.926021	2.622325	–1.631338
C	–4.376594	3.698024	–0.966196
C	–2.959344	3.799984	–0.834188
C	–2.125095	2.836997	–1.368232
C	–0.321805	0.764498	–2.491320
N	0.126674	0.098429	–1.247309
C	0.803981	0.706871	–0.276400
C	1.255595	0.331993	1.018208
C	1.868631	1.654860	1.273912
C	1.401577	2.072347	–0.124848
N	1.133630	–0.799520	1.753311
O	2.467604	2.186573	2.211559
O	1.451126	3.086930	–0.820852
C	1.780584	–0.989928	2.992051
C	1.043372	–1.326397	4.140920
C	1.665246	–1.536903	5.374529
C	3.053377	–1.390037	5.483320
C	3.809455	–1.055617	4.353420
C	3.176619	–0.876429	3.120019
H	0.034410	1.795680	–2.451717
H	–0.187578	–0.859744	–1.112279
H	0.465020	–1.511324	1.468967
F	–0.299530	–1.443054	4.054710
F	0.934774	–1.854976	6.461497
F	5.148449	–0.938124	4.453224
F	3.932537	–0.617762	2.034122
F	3.660653	–1.578242	6.669651
H	–1.051589	2.956238	–1.244235
H	–2.528228	4.650902	–0.304639
H	–5.017966	4.470461	–0.539965
H	–6.008109	2.527931	–1.740277
H	–5.744225	0.426183	–2.946375
H	–5.539570	–1.694057	–4.132379
H	–4.132404	–3.527422	–5.055273
H	–1.637641	–3.413303	–4.835253

H	–0.558081	–1.521412	–3.743241
H	0.185971	0.292856	–3.340252
Compound		**4**	
Atom	X	Y	Z
C	–4.682505	3.551152	–0.110009
C	–5.188394	2.309464	–0.416850
C	–4.437602	1.115413	–0.165935
C	–3.120999	1.205775	0.460279
C	–2.634146	2.534851	0.701925
C	–3.381814	3.661451	0.440718
C	–4.923090	–0.162565	–0.484288
C	–4.186114	–1.344118	–0.298437
C	–2.877446	–1.238910	0.343233
C	–2.398207	0.025092	0.789468
C	–4.682382	–2.627174	–0.696255
C	–3.943765	–3.771545	–0.503281
C	–2.658622	–3.683951	0.084027
C	–2.148441	–2.467093	0.482240
C	–1.187335	0.113422	1.708760
N	0.078616	0.244543	0.963597
C	1.235318	–0.261702	1.389478
C	2.563272	–0.258808	0.889991
C	3.072086	–1.078026	2.014326
C	1.641125	–1.085156	2.572838
N	3.131086	0.265939	–0.223261
O	4.160681	–1.555612	2.338914
O	1.062141	–1.568616	3.543997
C	4.520671	0.255887	–0.460587
C	5.042158	–0.293814	–1.644845
C	6.414583	–0.299240	–1.907612
C	7.301775	0.233142	–0.964274
C	6.806852	0.786251	0.222865
C	5.429264	0.811437	0.458260
F	4.198196	–0.836872	–2.549153
F	6.888465	–0.835933	–3.049383
F	7.658746	1.320597	1.120340
F	4.972731	1.406392	1.578724
F	8.626600	0.220340	–1.201675
F	–0.885164	–2.492118	0.968422
F	–1.929960	–4.807387	0.215365
F	–4.409798	–4.974753	–0.884228
F	–5.888137	–2.761522	–1.289690
F	–6.165667	–0.261333	–1.004355
F	–6.416513	2.261665	–0.976077
F	–5.388235	4.670906	–0.351015
F	–2.874999	4.887901	0.661675
F	–1.367158	2.755057	1.137480
H	–1.112732	–0.777733	2.331458
H	–1.303229	0.960328	2.391881
H	0.079987	0.883281	0.172778
H	2.533798	0.575181	–0.986793
Compound		**5**	
Atom	X	Y	Z
C	–3.429501	–2.397311	–4.804221
C	–4.271286	–1.320206	–4.561872
C	–3.883017	–0.263182	–3.670597
C	–2.564229	–0.302318	–3.043434
C	–1.770562	–1.471976	–3.273119
C	–2.186756	–2.484373	–4.132988
C	–4.725223	0.841115	–3.398258
C	–4.395483	1.835887	–2.445914
C	–3.067539	1.793594	–1.840596

C	–2.135810	0.796608	–2.237980
C	–5.304635	2.883976	–2.084929
C	–4.953922	3.851567	–1.166220
C	–3.679237	3.799465	–0.549741
C	–2.781947	2.784567	–0.834119
C	–0.656023	1.009872	–1.987943
N	–0.167564	0.283937	–0.774675
C	1.157806	0.223928	–0.505803
C	1.908206	–0.102452	0.658596
C	3.203466	0.041581	–0.091443
C	2.372731	0.365299	–1.338175
N	1.474986	–0.404643	1.898696
O	4.405248	–0.049646	0.151279
O	2.620910	0.623634	–2.517710
C	2.197648	–0.719151	3.076065
C	1.444316	–0.999183	4.234431
C	2.095740	–1.317257	5.431669
C	3.498013	–1.359877	5.487294
C	4.239447	–1.079337	4.328623
C	3.602907	–0.758457	3.121820
H	–0.436468	2.075321	–1.877109
H	–0.793751	0.395240	0.023173
H	0.464638	–0.412840	2.024841
H	0.353874	–0.968048	4.197626
H	1.502054	–1.532035	6.321030
H	5.329693	–1.108667	4.357260
H	4.189198	–0.543686	2.230618
H	4.004965	–1.608175	6.420147
O	–1.633014	2.692495	–0.082191
H	–1.697937	3.376315	0.616874
O	–3.411424	4.684886	0.498139
H	–2.950700	5.474850	0.152564
O	–5.871336	4.825710	–0.854888
H	–5.533548	5.326070	–0.085027
O	–6.573079	2.902878	–2.650981
H	–7.089201	3.644171	–2.279466
O	–5.898703	0.901841	–4.117399
H	–6.467259	1.635696	–3.783463
O	–5.484379	–1.395922	–5.214203
H	–5.991252	–0.577209	–5.008724
O	–3.797770	–3.420293	–5.641976
H	–4.687365	–3.200343	–5.985590
O	–1.428460	–3.609444	–4.312619
H	–0.649597	–3.511583	–3.724710
O	–0.554687	–1.744667	–2.663123
H	–0.502405	–1.307157	–1.780079
H	–0.072007	0.637599	–2.834319

Compound		**6**	
Atom	X	Y	Z
C	–3.525403	–2.753686	–4.502273
C	–4.346489	–1.785034	–3.965299
C	–3.800819	–0.626388	–3.321650
C	–2.357325	–0.459289	–3.246644
C	–1.544878	–1.500023	–3.813598
C	–2.108306	–2.606632	–4.418536
C	–4.639064	0.345719	–2.753376
C	–4.121134	1.476751	–2.101583
C	–2.680847	1.661170	–2.022462
C	–1.820875	0.695983	–2.614799
C	–4.992052	2.448166	–1.508262
C	–4.485448	3.551078	–0.853755
C	–3.073115	3.735174	–0.765872

C	–2.201257	2.824826	–1.331455
C	–0.318083	0.865231	–2.517709
N	0.195430	0.242457	–1.275106
C	0.872557	0.894706	–0.337855
C	1.401870	0.538312	0.943415
C	2.015959	1.864403	1.115520
C	1.407400	2.284360	–0.209710
N	1.333379	–0.600457	1.661331
O	2.780680	2.384086	1.953717
O	1.371920	3.307766	–0.896631
C	1.762819	–0.819343	3.006296
C	0.840290	–1.448398	3.875439
C	1.235296	–1.827684	5.168958
C	2.536317	–1.534693	5.609118
C	3.430744	–0.856510	4.771325
C	3.055979	–0.497027	3.468459
H	–3.951271	–3.632890	–4.987183
H	–5.432364	–1.884668	–4.015414
H	–0.459416	–1.432360	–3.767903
H	–1.461693	–3.379099	–4.837060
H	–5.721758	0.214208	–2.811140
H	–6.069651	2.291055	–1.584138
H	–5.156868	4.282819	–0.402783
H	–2.675823	4.607808	–0.245303
H	–1.133188	3.007172	–1.241136
H	0.195979	0.409607	–3.371180
H	–0.019437	1.915346	–2.498917
H	–0.071745	–0.726739	–1.114893
H	0.944968	–1.416149	1.190515
O	–0.447542	–1.751864	3.487413
H	–0.699307	–1.164267	2.748948
O	0.330461	–2.459042	5.990413
H	0.764906	–2.611310	6.852282
O	2.860783	–1.908748	6.893745
H	3.775140	–1.624060	7.084144
O	4.678936	–0.556163	5.267692
H	5.151877	–0.075539	4.555564
O	4.019000	0.125446	2.701281
H	3.681128	1.040380	2.467884

Compound		**7**	
Atom	X	Y	Z
C	–2.906219	–2.196999	–5.196016
C	–3.887728	–1.249688	–4.938403
C	–3.707506	–0.254348	–3.918366
C	–2.452483	–0.211972	–3.172604
C	–1.509503	–1.257291	–3.431740
C	–1.724804	–2.216231	–4.416608
C	–4.696627	0.714695	–3.627223
C	–4.569929	1.637648	–2.560417
C	–3.303326	1.680609	–1.836224
C	–2.228447	0.837436	–2.230346
C	–5.624600	2.537271	–2.195486
C	–5.471640	3.439157	–1.162575
C	–4.257681	3.464950	–0.432615
C	–3.224343	2.590378	–0.722074
C	–0.810584	1.190126	–1.824088
N	–0.347160	0.445189	–0.615095
C	0.949504	0.427459	–0.263399
C	1.648453	0.028504	0.913091
C	2.959460	0.230340	0.260769
C	2.222384	0.700794	–0.990114
N	1.222482	–0.378239	2.123613

O	4.142448	0.014522	0.574453
O	2.535886	1.101269	–2.110379
C	2.006217	–0.613130	3.295718
C	1.564328	–0.000491	4.491621
C	2.197081	–0.296437	5.710447
C	3.298692	–1.167387	5.725153
C	3.774676	–1.727446	4.532462
C	3.134042	–1.459573	3.314207
H	–0.728207	2.262791	–1.625829
H	–1.038362	0.422767	0.134832
H	0.226466	–0.572955	2.217587
O	–2.138201	2.551811	0.122336
H	–2.340206	3.149932	0.871839
O	–4.188110	4.261789	0.713118
H	–3.806330	5.132840	0.487004
O	–6.521309	4.270923	–0.856745
H	–6.315381	4.725305	–0.015184
O	–6.832119	2.475881	–2.878991
H	–7.462099	3.115242	–2.493863
O	–5.804625	0.716286	–4.445037
H	–6.482399	1.346448	–4.102935
O	–5.020929	–1.389368	–5.711387
H	–5.639578	–0.659268	–5.479427
O	–3.076209	–3.162970	–6.155809
H	–3.953394	–3.009594	–6.561873
O	–0.827542	–3.227734	–4.623403
H	–0.121513	–3.109871	–3.952912
O	–0.325211	–1.450474	–2.730828
H	–0.432728	–1.164667	–1.796561
O	3.642447	–2.092502	2.197265
H	3.977009	–1.386745	1.574593
O	4.882828	–2.540611	4.599100
H	5.073255	–2.827686	3.681056
O	3.892797	–1.402323	6.944286
H	4.653383	–2.000938	6.815624
O	1.738077	0.291912	6.865519
H	2.311226	–0.002908	7.599883
O	0.490744	0.863303	4.523975
H	0.356632	1.229399	3.628369
H	–0.113909	0.947138	–2.630385

Compound		NO_3^-	
Atom	X	Y	Z
N	–2.251342	–1.178709	0.657890
O	–2.290359	–0.033740	1.206973
O	–3.325755	–1.731703	0.265300
O	–1.137923	–1.770462	0.501226

Compound		$\mathbf{5}_{OH}\cdots Cl^-$	
Atom	X	Y	Z
C	–4.001083	–2.843246	–3.399717
C	–4.676559	–1.655216	–3.228476
C	–3.964277	–0.442466	–2.958326
C	–2.506219	–0.429615	–2.877569
C	–1.854557	–1.707898	–3.090968
C	–2.582361	–2.862677	–3.331598
C	–4.679747	0.746778	–2.748455
C	–4.041142	1.946833	–2.412538
C	–2.592145	1.972725	–2.291573
C	–1.837305	0.792232	–2.561558
C	–4.802203	3.138466	–2.173603
C	–4.184801	4.313796	–1.804837
C	–2.766407	4.343736	–1.652267
C	–1.998919	3.219588	–1.888422

C	–0.314725	0.870097	–2.499136
N	0.229987	0.267502	–1.267733
C	0.846548	0.935116	–0.299062
C	1.411699	0.525273	0.954123
C	1.837197	1.920892	1.266466
C	1.255983	2.344171	–0.073016
N	1.466641	–0.714953	1.482580
O	2.419851	2.515516	2.183750
O	1.181965	3.405040	–0.708380
C	1.994318	–1.148823	2.718352
C	1.948423	–2.534415	2.986177
C	2.448567	–3.030114	4.195750
C	2.998312	–2.159068	5.150730
C	3.039736	–0.782299	4.876832
C	2.542537	–0.268346	3.671286
H	0.031106	1.902981	–2.531801
H	0.126104	–0.747166	–1.181879
H	1.092133	–1.473459	0.889415
H	1.522443	–3.211371	2.244683
H	2.407039	–4.103068	4.389692
H	3.463581	–0.092733	5.608990
H	2.584585	0.800715	3.468818
H	3.387422	–2.547049	6.092816
Cl	0.401430	–3.156541	–0.489412
H	–2.278402	5.268130	–1.338810
H	–4.771823	5.214679	–1.620762
H	–5.887222	3.087847	–2.284007
H	–5.768620	0.728170	–2.831301
H	–5.765680	–1.615300	–3.279596
H	–4.542194	–3.770333	–3.593716
H	–2.039534	–3.797653	–3.476156
O	–0.478397	–1.780018	–3.056382
H	–0.200928	–2.499694	–2.424513
H	0.129212	0.349016	–3.350862
H	–0.926144	3.297291	–1.732343

Compound		$\mathbf{5}_{OH}\cdots Br^-$	
Atom	X	Y	Z
C	–3.809319	–2.601976	–4.531628
C	–4.554420	–1.497569	–4.179542
C	–3.975098	–0.442075	–3.403554
C	–2.574718	–0.510818	–2.994766
C	–1.894288	–1.764454	–3.260671
C	–2.476905	–2.738398	–4.051835
C	–4.748546	0.672423	–3.038805
C	–4.207575	1.742623	–2.310444
C	–2.790509	1.736434	–1.998533
C	–1.980004	0.638364	–2.401401
C	–5.017739	2.852332	–1.902577
C	–4.469363	3.917228	–1.218933
C	–3.075114	3.921321	–0.911964
C	–2.262350	2.872205	–1.296214
C	–0.473699	0.783332	–2.270381
N	–0.028155	0.479387	–0.900655
C	1.095839	0.914950	–0.341652
C	1.775591	0.515342	0.851999
C	2.816547	1.567679	0.665854
C	2.088419	1.983045	–0.612082
N	1.448939	–0.494412	1.685534
O	3.828460	1.962198	1.259393
O	2.256295	2.837509	–1.491324
C	2.065369	–0.926957	2.877235
C	1.522268	–2.072070	3.498715

C	2.082091	–2.552144	4.687802
C	3.180773	–1.900306	5.272232
C	3.713540	–0.760421	4.648022
C	3.165316	–0.265881	3.456533
H	–0.169433	1.808796	–2.508121
H	–0.504491	–0.314505	–0.448512
H	0.641659	–1.065975	1.391922
H	0.669404	–2.578124	3.043671
H	1.655271	–3.439072	5.158586
H	4.566927	–0.244189	5.091049
H	3.588515	0.615269	2.976122
H	3.615110	–2.275453	6.199585
Br	–1.222885	–2.286600	0.444992
H	–1.209307	2.899064	–1.024500
H	–2.648024	4.761228	–0.362062
H	–5.094521	4.756107	–0.909987
H	–6.081445	2.834955	–2.147613
H	–5.798329	0.707359	–3.338055
H	–5.597648	–1.403622	–4.485270
H	–4.245890	–3.397866	–5.136520
H	–1.912914	–3.651837	–4.242440
O	–0.623548	–2.023961	–2.774313
H	–0.682267	–2.087035	–1.782526
H	0.036774	0.113597	–2.969383

Compound		$\mathbf{6}_{OH^{\cdots}}Cl^{-}$	
Atom	X	Y	Z
C	–3.599140	–2.787160	–4.307737
C	–4.385051	–1.768690	–3.811845
C	–3.798117	–0.599020	–3.226696
C	–2.349391	–0.475437	–3.168103
C	–1.575168	–1.567874	–3.688961
C	–2.177410	–2.682597	–4.238371
C	–4.600935	0.424929	–2.699708
C	–4.041363	1.566975	–2.103731
C	–2.595207	1.706812	–2.041535
C	–1.770000	0.688699	–2.593223
C	–4.874895	2.593639	–1.550836
C	–4.327157	3.707779	–0.950443
C	–2.908825	3.848149	–0.878560
C	–2.072187	2.884020	–1.406990
C	–0.260454	0.811170	–2.506723
N	0.235125	0.238253	–1.238743
C	0.890492	0.936955	–0.313588
C	1.337506	0.617003	1.007574
C	1.896546	1.985911	1.200604
C	1.449864	2.309383	–0.220909
N	1.169978	–0.525827	1.697306
O	2.455435	2.614215	2.107954
O	1.495213	3.298643	–0.966038
C	1.685209	–0.866731	2.968877
C	1.013390	–1.850183	3.745727
C	1.515569	–2.176227	5.017551
C	2.662306	–1.552042	5.522948
C	3.336734	–0.595420	4.746952
C	2.854323	–0.267638	3.474934
H	–4.056563	–3.674457	–4.747331
H	–5.473998	–1.836488	–3.849813
H	–0.488345	–1.536705	–3.642741
H	–1.558803	–3.496337	–4.619584
H	–5.687811	0.326209	–2.745038
H	–5.957805	2.469640	–1.612575
H	–4.970898	4.481205	–0.529367

H	–2.478929	4.729231	–0.399594
H	–0.997878	3.032071	–1.329996
H	0.229003	0.295402	–3.340877
H	0.070535	1.851331	–2.550003
H	–0.101577	–0.700214	–0.987011
H	0.611910	–1.245623	1.208364
Cl	–0.731087	–2.626696	0.252410
O	–0.137421	–2.490073	3.361397
H	–0.316048	–2.450467	2.385283
H	0.981072	–2.926878	5.600667
H	3.031010	–1.821510	6.513500
H	4.240318	–0.113248	5.121123
H	3.371454	0.471398	2.867237

Compound		$\mathbf{6}_{OH^{\cdots}}Br^{-}$	
Atom	X	Y	Z
C	–3.432923	–2.845829	–4.164489
C	–4.130367	–2.015500	–3.313379
C	–3.532393	–0.824059	–2.787563
C	–2.174292	–0.471750	–3.170645
C	–1.488962	–1.372495	–4.054215
C	–2.094233	–2.517192	–4.533293
C	–4.227740	–0.012110	–1.879115
C	–3.641913	1.135262	–1.319690
C	–2.292749	1.512034	–1.708160
C	–1.578552	0.702294	–2.634252
C	–4.353014	1.935369	–0.366921
C	–3.774278	3.052935	0.197517
C	–2.451137	3.430472	–0.179120
C	–1.737488	2.688086	–1.100481
C	–0.106106	0.973036	–2.882408
N	0.658288	0.307037	–1.796203
C	1.230008	0.990557	–0.796107
C	1.520306	0.642228	0.557683
C	2.106102	1.986266	0.830944
C	1.799643	2.349155	–0.624563
N	1.206995	–0.475099	1.233146
O	2.585950	2.575659	1.804793
O	1.910905	3.358334	–1.333797
C	1.431573	–0.732870	2.608907
C	0.414002	–1.369913	3.367467
C	0.627332	–1.591921	4.739253
C	1.821440	–1.196188	5.354309
C	2.832098	–0.578572	4.599021
C	2.635738	–0.359652	3.230710
H	–3.894833	–3.754977	–4.551989
H	–5.151461	–2.257427	–3.011867
H	–0.461697	–1.170919	–4.350649
H	–1.539598	–3.182725	–5.196528
H	–5.238109	–0.295795	–1.575695
H	–5.366070	1.634298	–0.092774
H	–4.322620	3.650873	0.926724
H	–1.996835	4.317645	0.264781
H	–0.736368	3.018739	–1.364733
H	0.229742	0.580970	–3.846718
H	0.141386	2.036938	–2.871637
H	0.271305	–0.611213	–1.534724
H	0.639473	–1.163402	0.710170
Br	–0.941162	–2.397260	–0.380274
O	–0.810414	–1.734661	2.868182
H	–0.821730	–1.849294	1.881478
H	–0.166883	–2.072636	5.311269
H	1.963118	–1.377987	6.420447

H	3.770065	–0.278272	5.066597
H	3.409491	0.112626	2.627678
Compound		$\mathbf{6}_{OH}\cdots NO_3^-$	
Atom	X	Y	Z
C	–3.492154	–2.731485	–4.670021
C	–4.298128	–1.760260	–4.115392
C	–3.735381	–0.631735	–3.434121
C	–2.289448	–0.495032	–3.343112
C	–1.493727	–1.538631	–3.927981
C	–2.073216	–2.617279	–4.566706
C	–4.560543	0.333568	–2.836896
C	–4.026426	1.429307	–2.139333
C	–2.583977	1.586931	–2.051314
C	–1.735735	0.629167	–2.672201
C	–4.882123	2.391138	–1.509436
C	–4.358805	3.459932	–0.812386
C	–2.943898	3.619774	–0.719098
C	–2.086872	2.717515	–1.319321
C	–0.230470	0.770173	–2.550187
N	0.242312	0.170993	–1.284993
C	0.855957	0.857338	–0.321052
C	1.227440	0.532710	1.020693
C	1.808545	1.886107	1.240841
C	1.435994	2.220344	–0.201376
N	1.007575	–0.579140	1.741957
O	2.336393	2.494215	2.179248
O	1.528764	3.208780	–0.942853
C	1.565055	–0.863297	3.014656
C	0.782997	–1.559289	3.971680
C	1.349240	–1.868624	5.221826
C	2.658775	–1.481878	5.530587
C	3.430233	–0.785233	4.585134
C	2.883944	–0.490914	3.330899
H	0.286101	0.285222	–3.385710
H	0.085114	1.816486	–2.557186
H	–0.113604	–0.761804	–1.051993
H	0.427053	–1.303860	1.284740
N	–1.931544	–1.970792	0.525502
O	–2.136174	–1.383418	1.637059
O	–2.881458	–2.288908	–0.216537
O	–0.720565	–2.226914	0.173693
H	–0.408168	–1.499275	–3.862086
H	–1.438367	–3.394659	–4.994383
H	–3.931339	–3.589163	–5.181210
H	–5.385461	–1.837077	–4.176231
H	–5.645114	0.221813	–2.903239
H	–5.962149	2.253982	–1.590903
H	–5.019302	4.183495	–0.332720
H	–2.533019	4.466344	–0.166839
H	–1.016203	2.880096	–1.226538
H	3.476207	0.026540	2.578045
O	–0.502780	–1.965255	3.754281
H	–0.903118	–1.623293	2.910027
H	0.734812	–2.402654	5.947454
H	3.074937	–1.726526	6.508816
H	4.453593	–0.486964	4.814230
Compound		$\mathbf{7}_{OH}\cdots Cl^-$	
Atom	X	Y	Z
C	–3.788222	–2.839223	–3.410249
C	–4.513981	–1.673224	–3.310649
C	–3.862301	–0.429040	–3.031310
C	–2.413346	–0.357683	–2.862538

C	–1.709080	–1.617286	–3.001823
C	–2.377178	–2.804444	–3.255785
C	–4.632369	0.737163	–2.901350
C	–4.061028	1.969621	–2.563846
C	–2.624179	2.055179	–2.354848
C	–1.810231	0.898031	–2.542957
C	–4.879941	3.136774	–2.410330
C	–4.331623	4.345808	–2.042122
C	–2.928036	4.435075	–1.801519
C	–2.105707	3.335713	–1.953971
C	–0.295747	1.040386	–2.406110
N	0.232220	0.427455	–1.175269
C	0.654098	1.077003	–0.095084
C	1.112909	0.608960	1.176594
C	1.304127	1.999348	1.674479
C	0.883947	2.493404	0.293892
N	1.219583	–0.656789	1.625072
O	1.642664	2.542646	2.733399
O	0.779536	3.595535	–0.260412
C	1.803153	–1.092460	2.840187
C	1.370206	–2.316618	3.417840
C	1.921170	–2.728968	4.642517
C	2.893434	–1.957436	5.291543
C	3.343212	–0.763600	4.705333
C	2.808176	–0.344755	3.481588
H	0.005714	2.087375	–2.402502
H	0.199256	–0.592999	–1.164633
H	0.934485	–1.393431	0.961999
Cl	0.437644	–3.175866	–0.275071
H	–1.051112	3.458577	–1.722826
H	–2.495969	5.385623	–1.484422
H	–4.962330	5.227935	–1.923457
H	–5.953191	3.039837	–2.585564
H	–5.712255	0.674009	–3.051457
H	–5.598647	–1.674448	–3.427395
H	–4.282352	–3.790460	–3.611615
H	–1.795713	–3.723445	–3.342252
O	–0.334907	–1.635688	–2.875057
H	–0.070080	–2.437665	–2.361988
H	3.154255	0.577323	3.020430
H	4.115012	–0.164023	5.188864
H	3.306231	–2.297119	6.242287
H	1.566510	–3.665716	5.073553
O	0.384290	–3.108835	2.880932
H	0.355823	–3.068138	1.890013
H	0.206875	0.561850	–3.251696

Compound		$\mathbf{7}_{OH}{}^{\cdot\cdot}Br^-$	
Atom	X	Y	Z
C	–4.039827	–2.768665	–3.353390
C	–4.696002	–1.567511	–3.200326
C	–3.963596	–0.360769	–2.960485
C	–2.505301	–0.369968	–2.887758
C	–1.874620	–1.657885	–3.099957
C	–2.620822	–2.805901	–3.309268
C	–4.658257	0.845277	–2.777308
C	–3.999615	2.041382	–2.466418
C	–2.551131	2.043626	–2.341244
C	–1.818029	0.846219	–2.591787
C	–4.739163	3.251494	–2.254787
C	–4.100936	4.421789	–1.905942
C	–2.683306	4.427455	–1.742704
C	–1.936352	3.284262	–1.950668

C	–0.298386	0.888654	–2.487312
N	0.165493	0.287307	–1.224238
C	0.809871	0.937488	–0.260656
C	1.293966	0.524923	1.020181
C	1.890305	1.862795	1.283530
C	1.344048	2.311718	–0.068651
N	1.220473	–0.685160	1.605997
O	2.564024	2.390311	2.177695
O	1.367415	3.354101	–0.737350
C	1.646589	–1.036414	2.910214
C	2.121919	–2.352077	3.156310
C	2.578592	–2.685057	4.442703
C	2.558691	–1.743929	5.479443
C	2.064068	–0.451136	5.242470
C	1.600445	–0.108854	3.967192
H	0.077774	1.910764	–2.514989
H	–0.026010	–0.711022	–1.102722
H	0.761435	–1.420704	1.047673
Br	–0.038725	–3.169247	–0.246832
H	–0.863021	3.343536	–1.789276
H	–2.180259	5.347865	–1.441894
H	–4.671201	5.337473	–1.743777
H	–5.824393	3.219545	–2.369819
H	–5.747386	0.842864	–2.858019
H	–5.784810	–1.512872	–3.241950
H	–4.595550	–3.692089	–3.520887
H	–2.094526	–3.750843	–3.450588
O	–0.496221	–1.743468	–3.097447
H	–0.232379	–2.517330	–2.543702
H	1.210892	0.888265	3.773338
H	2.026533	0.285020	6.045860
H	2.918544	–2.025374	6.469918
H	2.951945	–3.696130	4.608313
O	2.231140	–3.325682	2.193452
H	1.610112	–3.196855	1.433537
H	0.164044	0.347035	–3.315696

Compound		$\mathbf{7}_{OH}{\cdots}NO_3^-$	
Atom	X	Y	Z
C	–3.785652	–2.745152	–4.305929
C	–4.504565	–1.671004	–3.826350
C	–3.843866	–0.529912	–3.264603
C	–2.390072	–0.492762	–3.216697
C	–1.687230	–1.639780	–3.721088
C	–2.359830	–2.726361	–4.244786
C	–4.580737	0.544799	–2.743623
C	–3.950413	1.656503	–2.161121
C	–2.498431	1.712954	–2.115286
C	–1.738765	0.642861	–2.662964
C	–4.717137	2.733079	–1.606753
C	–4.099551	3.817953	–1.020510
C	–2.674841	3.878421	–0.967889
C	–1.901536	2.863989	–1.498720
C	–0.224536	0.679864	–2.584293
N	0.237357	0.148013	–1.285269
C	0.919670	0.861574	–0.389521
C	1.302157	0.613853	0.965692
C	1.978939	1.936399	1.069282
C	1.594502	2.185617	–0.386780
N	1.025854	–0.422748	1.774545
O	2.569620	2.575806	1.947492
O	1.736617	3.106503	–1.203591
C	1.596896	–0.651625	3.052073

C	0.797341	–1.227126	4.072709
C	1.375438	–1.485620	5.328956
C	2.714633	–1.165017	5.581170
C	3.503735	–0.587140	4.572377
C	2.944717	–0.345193	3.312563
H	0.231788	0.092296	–3.388513
H	0.167047	1.695282	–2.682661
H	–0.178687	–0.735131	–0.971903
H	0.381380	–1.134599	1.388713
N	–2.047035	–1.646377	0.736331
O	–2.170723	–0.977550	1.813475
O	–3.038334	–1.913350	0.029517
O	–0.873749	–2.038843	0.382255
H	3.548991	0.078349	2.512194
O	–0.516365	–1.564087	3.911594
H	–0.920800	–1.243025	3.060719
H	0.747516	–1.926850	6.103716
H	3.139910	–1.368139	6.564951
H	4.549704	–0.341367	4.757459
H	–0.819807	2.952835	–1.439962
H	–2.189370	4.737666	–0.502594
H	–4.693008	4.629494	–0.597299
H	–5.806014	2.671108	–1.655275
H	–5.671938	0.508710	–2.778137
H	–5.595928	–1.672984	–3.856649
H	–4.298926	–3.611137	–4.725979
H	–1.794306	–3.583499	–4.613199
H	–0.600088	–1.674240	–3.683343

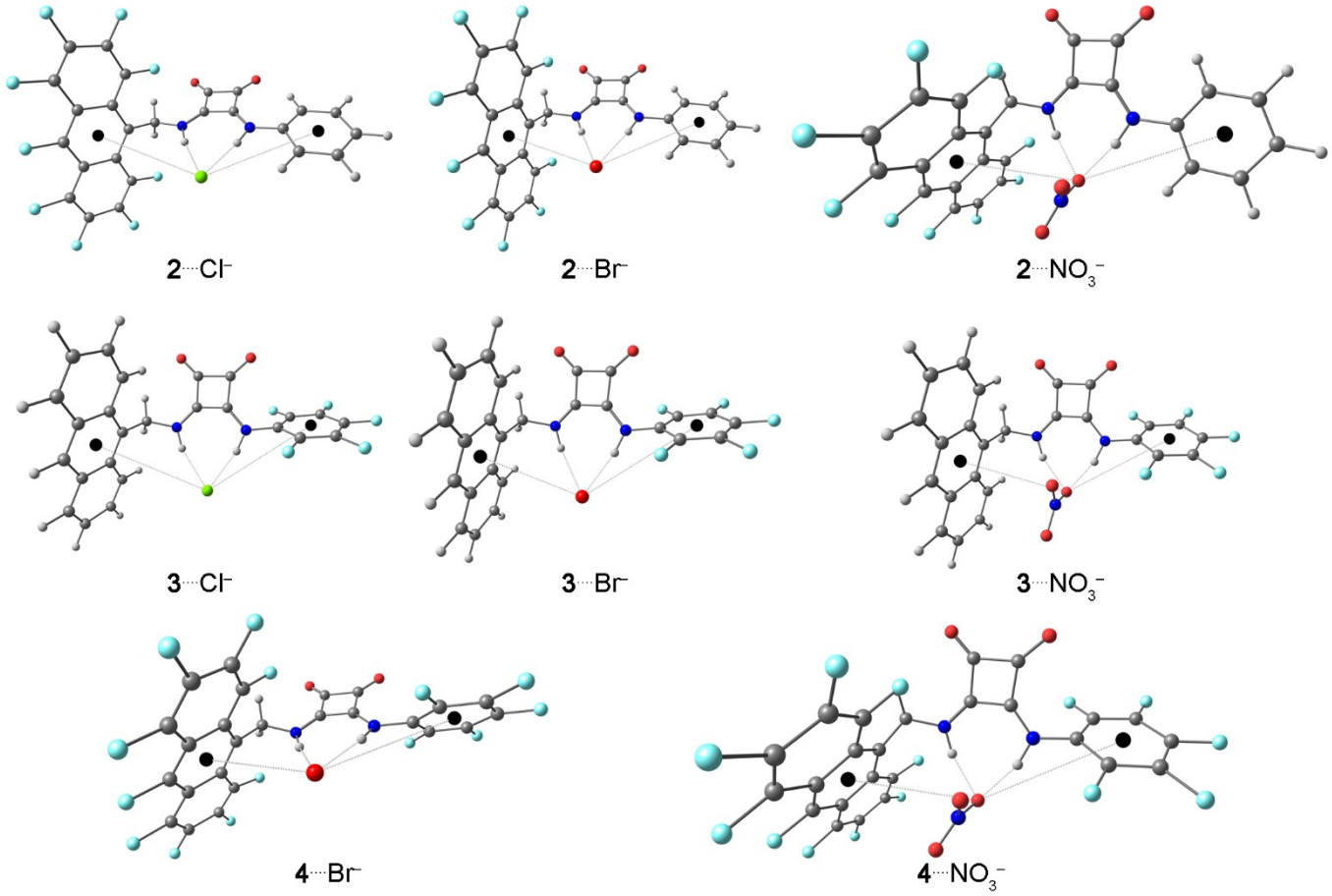

Figure S1. Optimized geometries of selected complexes: (**2** and **3**)···(Cl^-, Br^- and NO_3^-) and **4**···(Br^- and NO_3^-). Dotted lines were included to highlight the bond lengths of the main hydrogen bonds and anion–π interactions organized in the Table 1. Black dots represent the centroid of the aromatic ring in the anthracene and benzene structures. Atoms color code: H = white; C = gray; N = blue; O = red; F = light blue; Cl = green; and Br = light red.

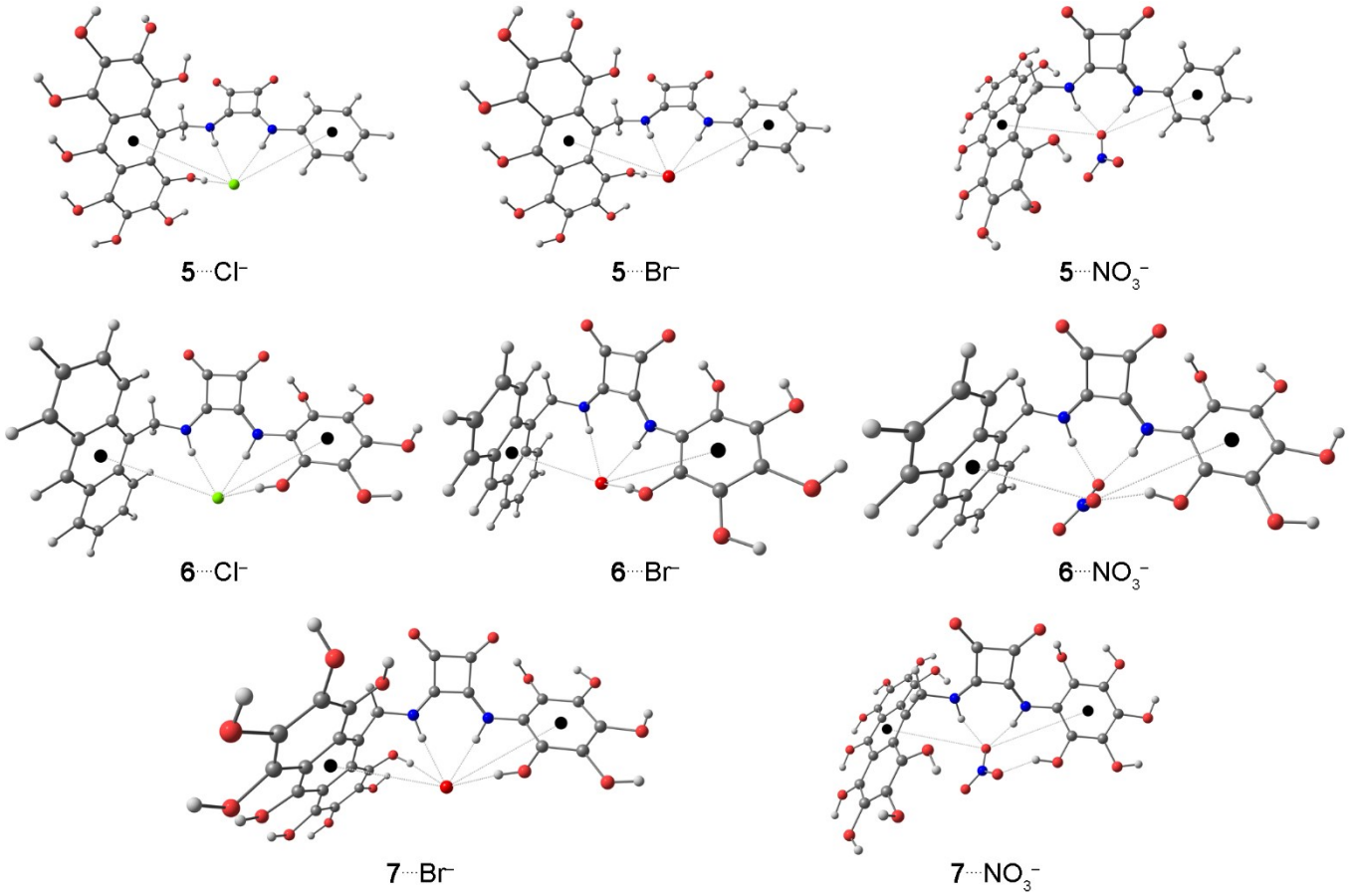

Figure S2. Optimized geometries of selected complexes: (**5** and **7**)···(Cl^-, Br^- and NO_3^-) and **7**···(Br^- and NO_3^-). Dotted lines were included to highlight the bond lengths of the main hydrogen bonds and anion–π interactions organized in the Table 1. Black dots represent the centroid of the aromatic ring in the anthracene and benzene structures. Atoms color code: H = white; C = gray; N = blue; O = red; Cl = green; and Br = light red.

Table S2. Selected APT atomic charges (a.u.) in the complexes studied.

Complex	$q_{A–H}$[a]	$q_{B–H}$[b]	$q_{O–H}$[c]	$q_{Total(H)}$[d]	q_{Anion}[e]	q_D[f]
1···Cl^-	0.452	0.481	–	0.933	–1.074	2.007
1···Br^-	0.459	0.491	–	0.951	–1.044	1.995
1···NO_3^-	0.406	0.454	–	0.860	–1.119	1.979
2···Cl^-	0.464	0.474	–	0.938	–1.076	2.014
2···Br^-	0.475	0.459	–	0.934	–1.048	1.982
2···NO_3^-	0.406	0.449	–	0.855	–1.117	1.972
3···Cl^-	0.446	0.577	–	1.023	–1.077	2.100
3···Br^-	0.461	0.59	–	1.051	–1.042	2.093
3···NO_3^-	0.392	0.535	–	0.927	–1.131	2.058
4···Cl^-	0.461	0.563	–	1.024	–1.079	2.103
4···Br^-	0.471	0.565	–	1.036	–1.051	2.087
4···NO_3^-	0.381	0.533	–	0.914	–1.123	2.037
5···Cl^-	0.406	0.424	0.638	1.468	–1.099	2.567
5···Br^-	0.437	0.446	0.611	1.494	–1.060	2.554
5···NO_3^-	0.392	0.502	–	0.894	–1.141	2.035
6···Cl^-	0.418	0.462	0.609	1.489	–1.085	2.574
6···Br^-	0.443	0.451	0.626	1.520	–1.028	2.548
6···NO_3^-	0.366	0.443	0.632	1.441	–1.055	2.496
7···Cl^-	0.398	0.422	1.160	1.980	–1.133	3.113
7···Br^-	0.437	0.421	1.156	2.014	–1.082	3.096
7···NO_3^-	0.380	0.463	0.654	1.497	–1.078	2.575

[a] APT charge related to hydrogen atom in the –NH group closer to the anthracene ring; [b] APT charge of the hydrogen atom in the –NH group closer to the benzene ring; [c] APT charge of the hydrogen atoms in the –OH groups closer to anion; [d] $q_{Total(H)} = q_{A–H} + q_{B–H} + q_{O–H}$; [e] APT charge of Cl^-, Br^-, and the oxygen atom of the NO_3^- anion in the closest position to the –NH groups; [f] $q_D = q_{A–H} + q_{B–H} + q_{O–H} – q_{Anion}$.

To evaluate the importance of the electrostatic interactions between the hydrogen atom of the groups –NH and –OH, in the receptors **1–7**, and the anions Cl^-, Br^- and NO_3^-, the APT atomic charges of: i) the hydrogen atom of the –NH group closer to anthracene ring, $q_{A\text{-}H}$; ii) the hydrogen atom of the –NH group closer to benzene ring, $q_{B\text{-}H}$; iii) the hydrogen atom of the –OH group closer to anion; and iv) Cl^-, Br^-, and of the oxygen atom of the NO_3^- anion in the closest position to –NH/–OH groups, q_{Anion}, are organized in the Table S2. The values of: $q_D = q_{A\text{-}H} + q_{B\text{-}H} + q_{O\text{-}H} - q_{Anion}$ (Table S2), will be used as base to establish the strength of these local electrostatic interactions and will be compared with the values obtained to ΔV_{elstat} energy in the bonds (**1–7**)···(Cl^-, Br^- and NO_3^-).

The H → F substitutions in the anthracene ring (**1** → **2**) increase the value of q_D from **1**···Cl^- to **2**···Cl^-. However, the opposite trend is visualized from **1**···Br^- and **1**···NO_3^- to **2**···Br^- and **2**···NO_3^-, respectively. It occurs because in **1**···Cl^- → **2**···Cl^- there is an increase in the value of $q_{A–H}$, which counterbalance the decrease in the value of $q_{B–H}$. However, in **1**···Br^- → **2**···Br^- and **1**···NO_3^- → **2**···NO_3^- there is not an relevant increase of $q_{A–H}$, which counterbalance the decrease in the value of $q_{B–H}$. These data show that the H → F substitutions favor only the electrostatic interaction anthracene–NH···Cl^-, in agreement with the more favorable ΔV_{elstat} energy in **2**···Cl^- compared to **1**···Cl^-. For Br^- and NO_3^- recognition, the H → F substitutions favor the anion–π interactions, which promote more favorable values of the ΔV_{elstat} component in **2**···Br^- and **2**···NO_3^- regarding to **1**···Br^- and **1**···NO_3^-, respectively. The H → F substitutions in the benzene ring (**1** → **3**) promote a relevant increase in the values of $q_{B–H}$ and are responsible by larger values of q_D and more stabilizing values of the ΔV_{elstat} term in the structures **3**···(Cl^-, Br^- and NO_3^-) regarding to **1**···(Cl^-, Br^- and NO_3^-). This same trend is observed when the H → F substitutions occur in the both rings: anthracene and benzene (**1** → **4**).

The –OH substituted structures (**5–7**)···(Cl^-, Br^- and NO_3^-) have larger values of q_D and more favorable values of the ΔV_{elstat} term compared to non–substituted complexes **1**···(Cl^-, Br^- and NO_3^-). The presence of –OH groups did not polarize the interactions –NH···(Cl^-, Br^- and NO_3^-), as can be observed by lower values of $q_{A–H}$ and $q_{B–H}$ in the complexes (**5–7**)···(Cl^-, Br^- and NO_3^-) regarding

to **1**···(Cl^-, Br^- and NO_3^-). Exceptionally, the presence of –OH groups in the anthracene ring of the complex **5**···NO_3^- polarizes the interaction benzene–O–H···NO_3^-. However, in general, the –OH groups provide the hydrogen atoms, which can establish electrostatic interactions with the anions Cl^-, Br^- and NO_3^-. It explains the larger values of q_D in the structures (**5**–**7**)···(Cl^-, Br^- and NO_3^-) than in the complexes **1**···(Cl^-, Br^- and NO_3^-). On the whole, the H → OH substitutions promote larger values of q_D and more attractive ΔV_{elstat} energy than H → F substitutions from the comparison of the structures (**5**–**7**)···(Cl^-, Br^- and NO_3^-) concerning to (**2**–**4**)···(Cl^-, Br^- and NO_3^-). As exception, the interaction **5**···NO_3^- appears with a less attractive value of the ΔV_{elstat} component than the bond **2**···NO_3^- due to the anion–π interaction between anthracene ring present in the receptor **2** and the anion NO_3^- and the absence of an –OH group in the receptor **5** with suitable orientation to interact with the anion NO_3^-, as highlighted from the discussion realized using the MEP surfaces.

The values of q_D in the interactions (**1**–**7**)···Cl^- are larger than in the bonds (**1**–**7**)···Br^-. It indicates that the local electrostatic interactions –NH···Cl^- are more favorable than the bonds –NH···Br^-. Overall, it agrees with the more attractive values of the ΔV_{elstat} component in the structures (**1**–**7**)···Cl^- regarding to complexes (**1**–**7**)···Br^-. The exceptions are the molecules **2**···Cl^- and **4**···Cl^- with less favorable values of the ΔV_{elstat} term in relation to complexes **2**···Br^- and **4**···Br^-, respectively. This trend, as mentioned in the analysis of the MEP surfaces, is, probably, due to the bromide anion preferentially interacting with the π–acid region presents in the receptors **2** and **4**, regarding to chloride anion. The bonds (**1**–**7**)···Cl^- show larger values of q_D and more attractive values of the ΔV_{elstat} energy compared to interactions (**1**–**7**)···NO_3^-. Here, the more favorable electrostatic interactions –NH···Cl^- than the bonds –NH···NO_3^- appear as decisive to establish the more attractive electrostatic interactions in the structures (**1**–**7**)···Cl^- concerning to compounds (**1**–**7**)···NO_3^-. The interactions (**1**–**7**)···Br^- show in relation to bonds (**1**–**7**)···NO_3^- the same tendency in relation to the comparison between the complexes (**1**–**7**)···Cl^- and (**1**–**7**)···NO_3^-, using the parameters q_D and ΔV_{elstat}.

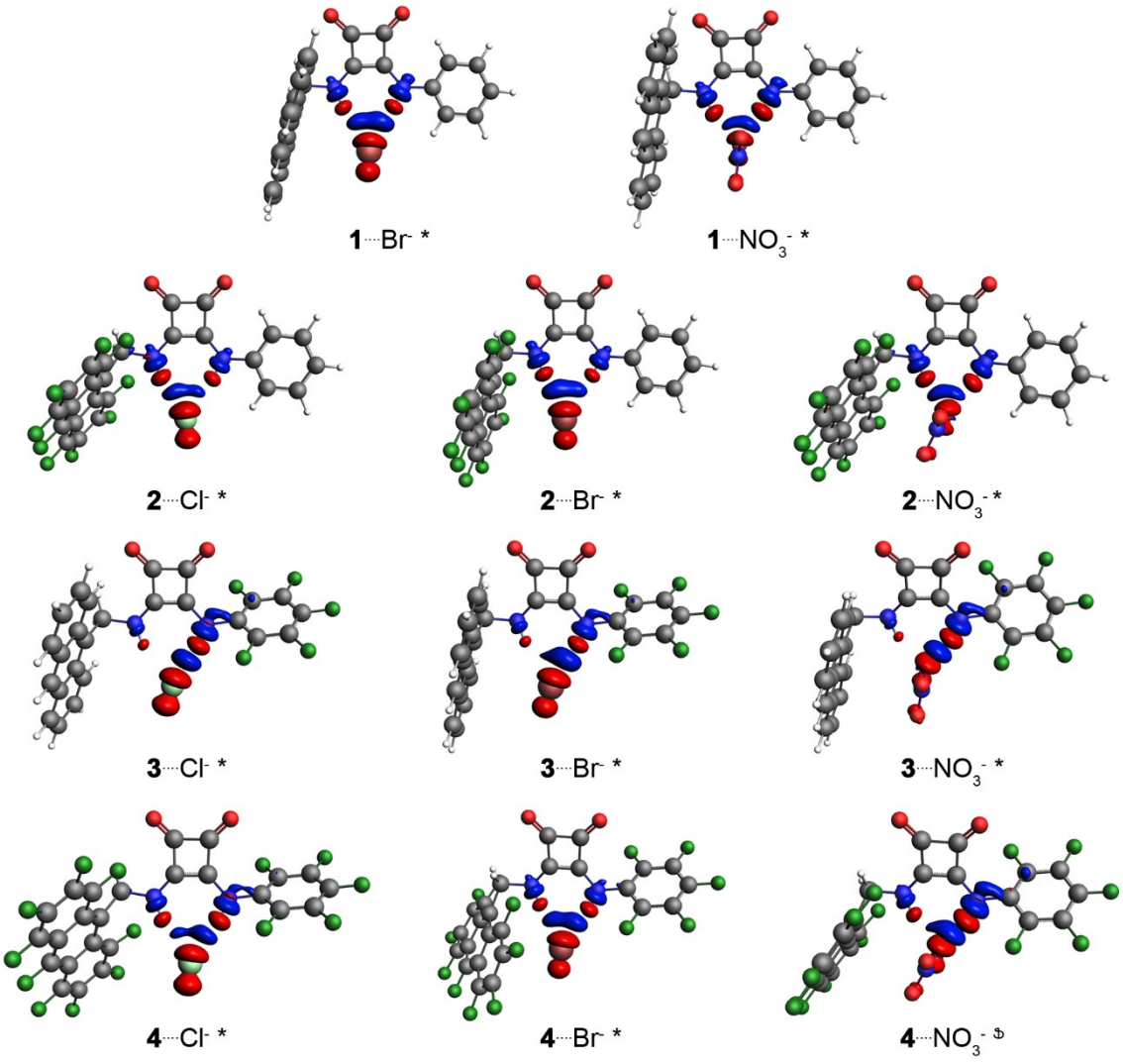

Figure S3. The first density deformation channel surface plots, $\Delta\rho_1$, related to interactions between the receptors (**1**–**4**) and anions (Cl^-, Br^- and NO_3^-). Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is: * = 0.002; and = 0.015 a.u. Atoms color code: H = white; C = gray; N = blue; O = red; F = green; Cl = light green; and Br = brown.

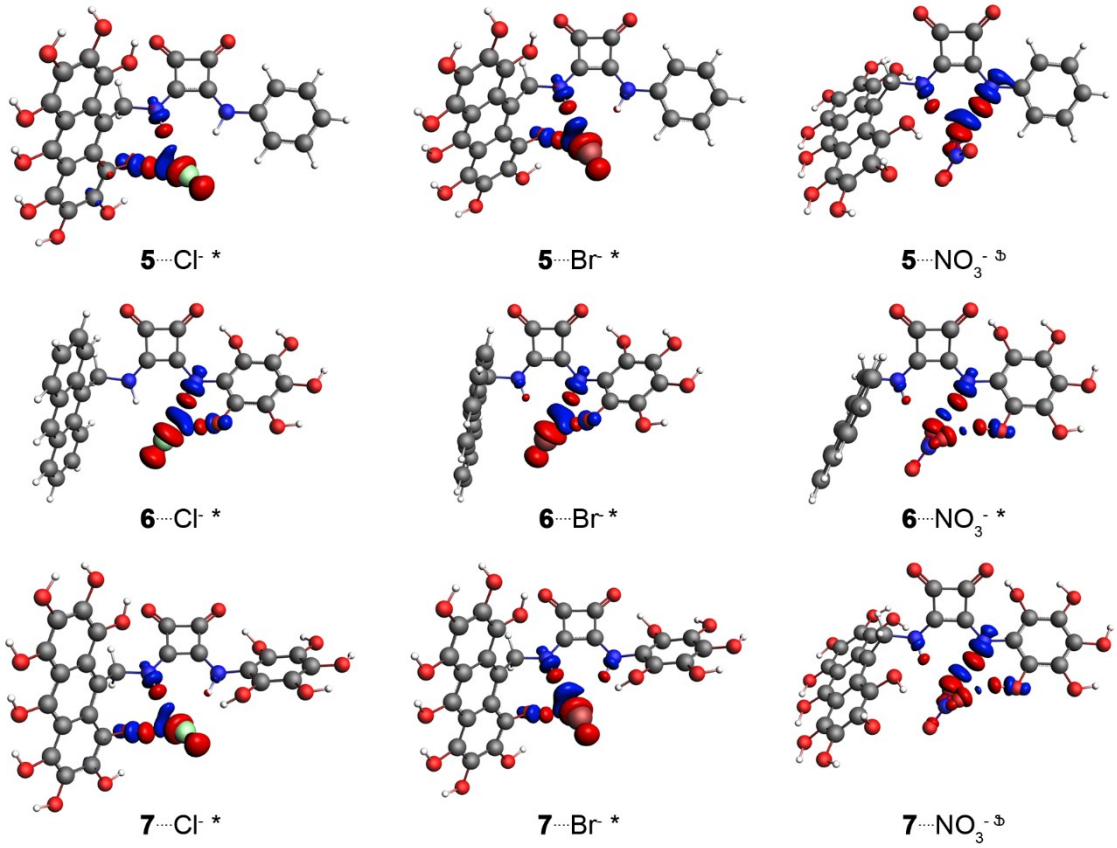

Figure S4. The first density deformation channel surface plots, $\Delta\rho_1$, related to interactions between the receptors (**5**–**7**) and anions (Cl^-, Br^- and NO_3^-). Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is: * = 0.002; and Φ = 0.015 a.u. Atoms color code: H = white; C = gray; N = blue; O = red; Cl = light green; and Br = brown.

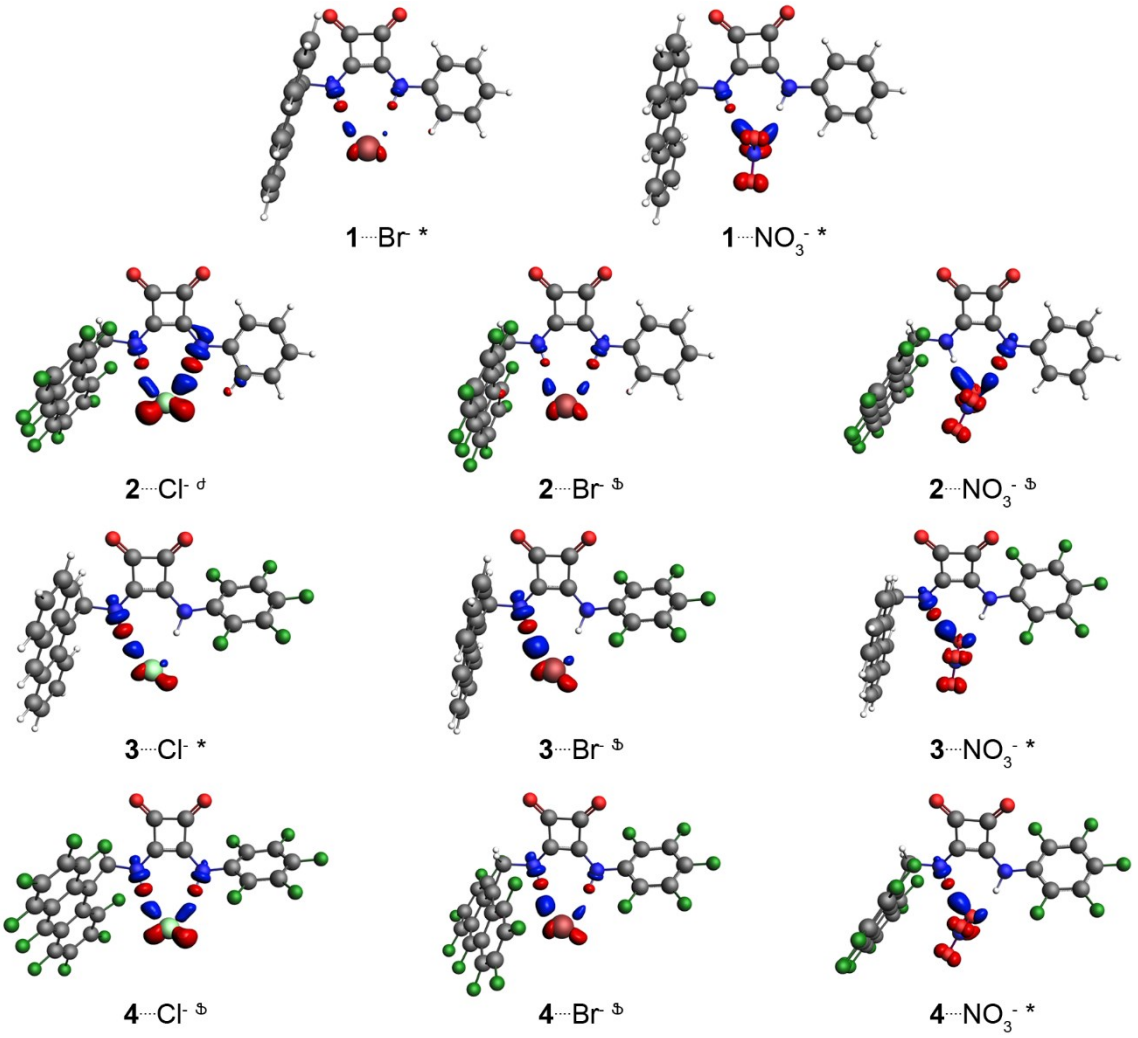

Figure S5. The second density deformation channel surface plots, $\Delta\rho_2$, related to interactions between the receptors (**1–4**) and anions (Cl^-, Br^- and NO_3^-). Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is: * = 0.002; ∂ = 0.015; and Ð = 0.010 a.u. Atoms color code: H = white; C = gray; N = blue; O = red; F = green; Cl = light green; and Br = brown.

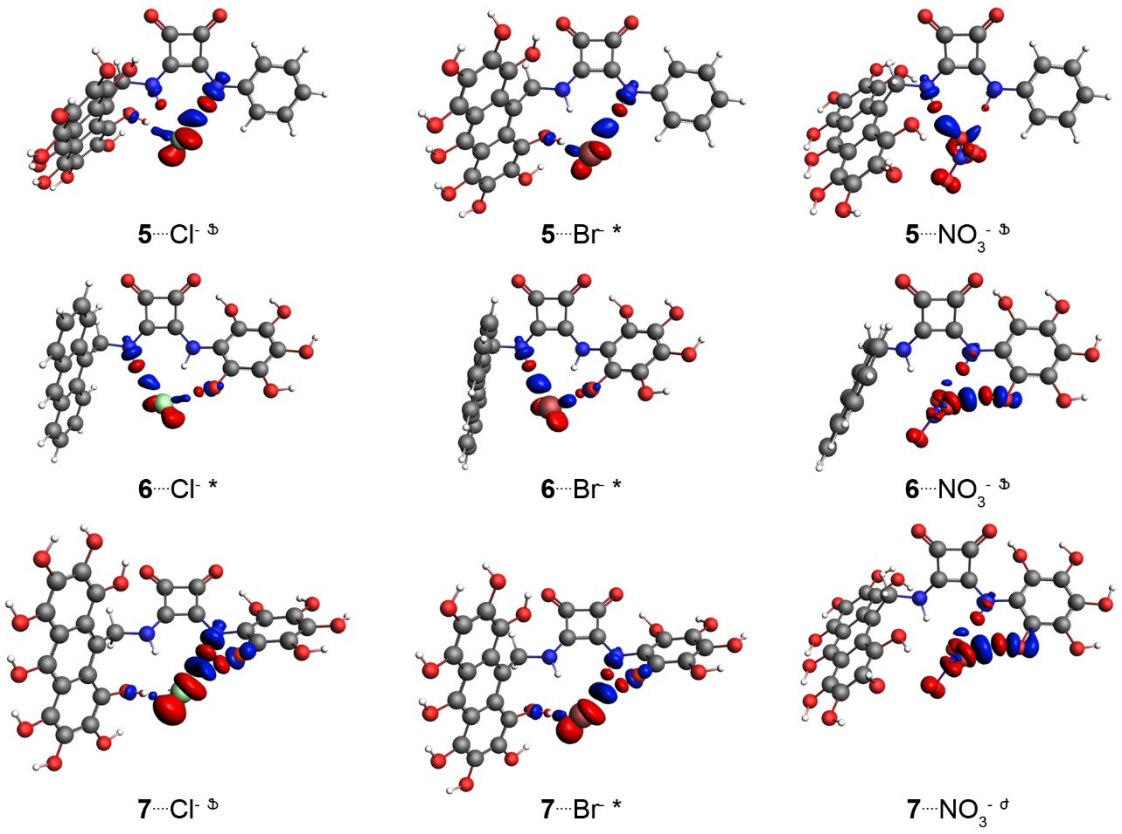

Figure S6. The second density deformation channel surface plots, $\Delta\rho_2$, related to interactions between the receptors (**5**–**7**) and anions (Cl^-, Br^- and NO_3^-). Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is: * = 0.002; Φ = 0.015; and σ = 0.010 a.u. Atoms color code: H = white; C = gray; N = blue; O = red; Cl = light green; and Br = brown.

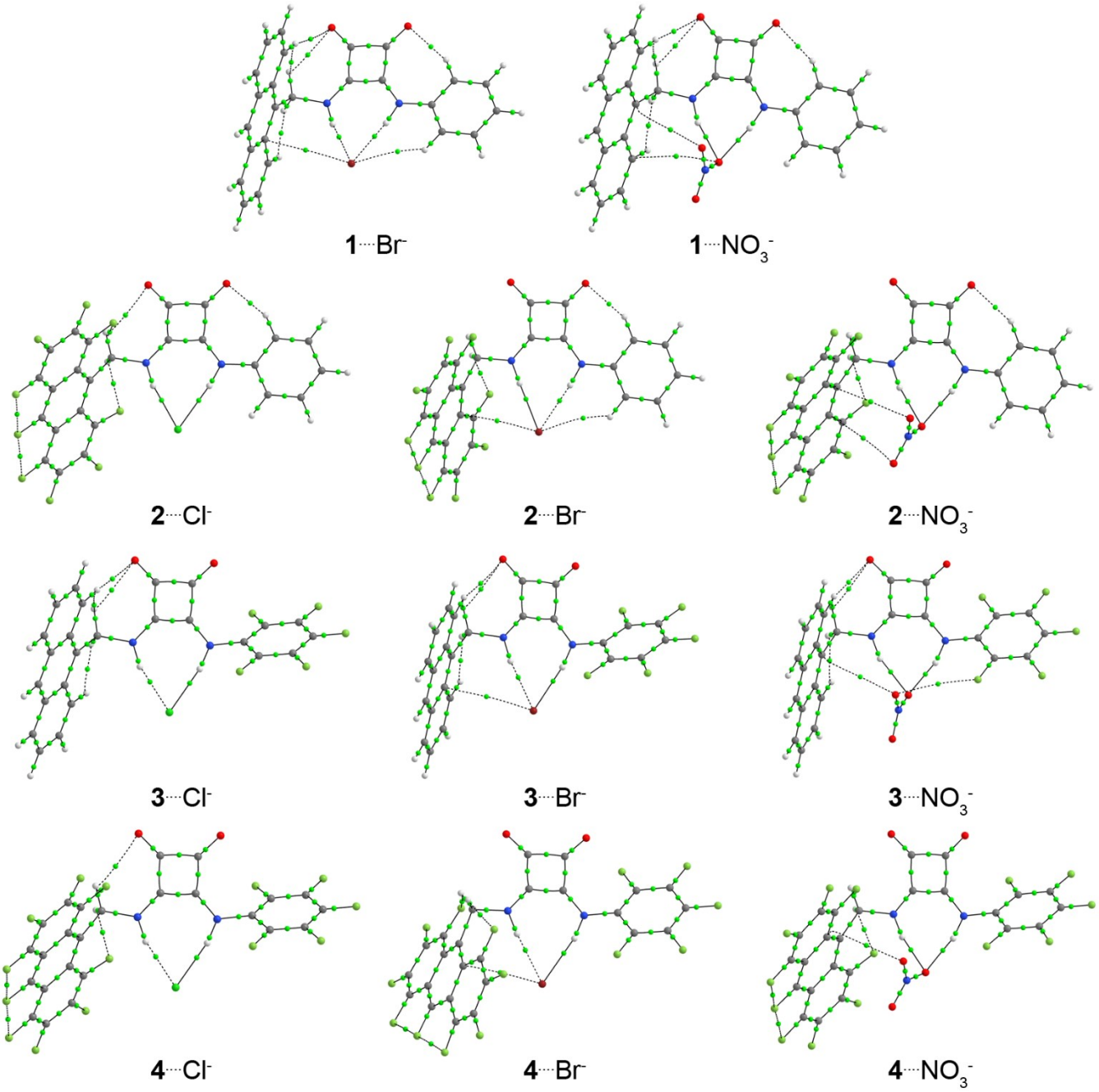

Figure S7. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points) related to interactions between the receptors (**1–4**) and anions (Cl^-, Br^- and NO_3^-). Atoms color code: H = white; C = gray; N = blue; O = red; F = green; Cl = light green; and Br = brown.

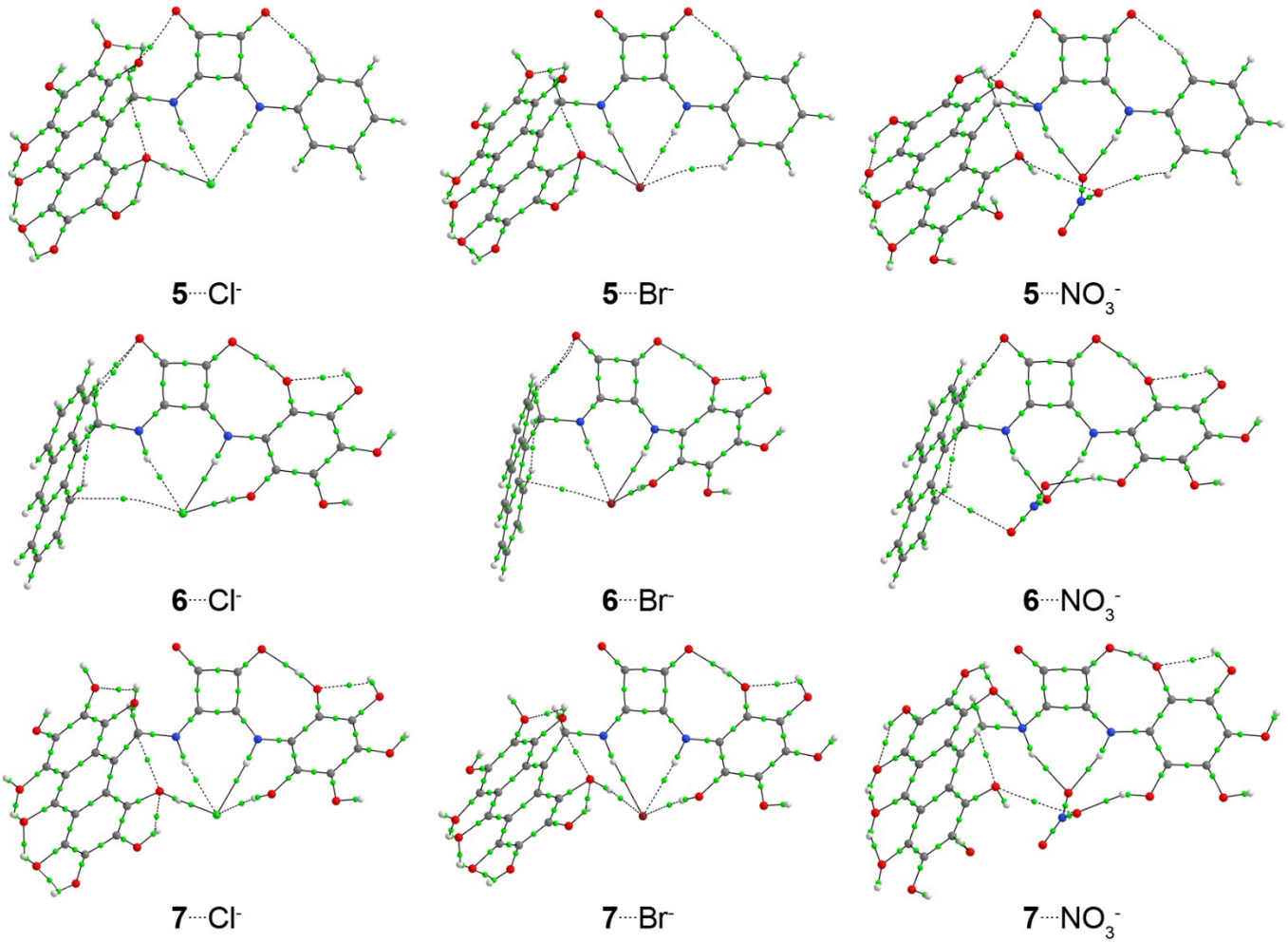

Figure S8. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points) related to interactions between the receptors (**5**–**7**) and anions (Cl^-, Br^- and NO_3^-). Atoms color code: H = white; C = gray; N = blue; O = red; Cl = light green; and Br = brown.

Table S3. Ratio between the kinetic energy density, G_b, and potential energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at BCPs related to interactions between the receptors (**1**–**4**) and anions (Cl^-, Br^- and NO_3^-). The values of all the parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
1···Cl^-	C···Cl^-	1.304	0.002
	N(1)–H(1)···Cl^- [a]	0.965	0.024
	N(2)–H(2)···Cl^- [b]	0.941	0.027
1···Br^-	C···Br^-	1.229	0.005
	N(1)–H(1)···Br^- [a]	0.978	0.024
	N(2)–H(2)···Br^- [b]	0.960	0.025
	C–H···Br^-	1.323	0.006
1···NO_3^-	C···O^-	1.389	0.002
		1.392	0.003
	N(1)–H(1)···O^- [a]	0.957	0.029
	N(2)–H(2)···O^- [b]	0.949	0.032
2···Cl^-	N(1)–H(1)···Cl^- [a]	0.947	0.026
	N(2)–H(2)···Cl^- [b]	0.956	0.025
2···Br^-	C···Br^-	1.238	0.007
	N(1)–H(1)···Br^- [a]	0.941	0.027
	N(2)–H(2)···Br^- [b]	0.999	0.021
	C–H···Br^-	1.336	0.006
2···NO_3^-	C···O^-	1.425	0.002
		1.425	0.002
	N(1)–H(1)···O^- [a]	0.960	0.033
	N(2)–H(2)···O^- [b]	0.945	0.030
3···Cl^-	N(1)–H(1)···Cl^- [a]	0.986	0.023
	N(2)–H(2)···Cl^- [b]	0.912	0.031
3···Br^-	C···Br^-	1.228	0.005
	N(1)–H(1)···Br^- [a]	0.988	0.023
	N(2)–H(2)···Br^- [b]	0.923	0.029
3···NO_3^-	C···O^-	1.364	0.003
	N(1)–H(1)···O^- [a]	0.960	0.027
	N(2)–H(2)···O^- [b]	0.957	0.036
	C–F···O^-	1.681	0.002
4···Cl^-	N(1)–H(1)···Cl^- [a]	0.963	0.025
	N(2)–H(2)···Cl^- [b]	0.924	0.029
4···Br^-	C···Br^-	1.243	0.007
	N(1)–H(1)···Br^- [a]	0.965	0.025
	N(2)–H(2)···Br^- [b]	0.954	0.025
4···NO_3^-	C···O^-	1.334	0.003
	N(1)–H(1)···O^- [a]	0.964	0.028
	N(2)–H(2)···O^- [b]	0.955	0.034

[a] BCP related to –NH group closer to anthracene ring; [b] BCP related to –NH group closer to benzene ring.

Table S4. Ratio between the kinetic energy density, G_b, and potential energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at BCPs related to interactions between the receptors (**5**–**7**) and anions (Cl^-, Br^- and NO_3^-). The values of all the parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
5···Cl^-	O–H···Cl^-	0.899	0.032
	N(1)–H(1)···Cl^-[a]	0.979	0.023
	N(2)–H(2)···Cl^-[b]	1.011	0.021
5···Br^-	O–H···Br^-	0.928	0.028
	N(1)–H(1)···Br^-[a]	0.960	0.026
	N(2)–H(2)···Br^-[b]	1.008	0.021
	C–H···Br^-	1.354	0.005
5···NO_3^-	C–HO···O^-	1.154	0.008
	N(1)–H(1)···O^-[a]	0.976	0.026
	N(2)–H(2)···O^-[b]	0.950	0.035
	C–H···O^-	1.458	0.003
6···Cl^-	C···Cl^-	1.321	0.002
	N(1)–H(1)···Cl^-[a]	1.018	0.020
	N(2)–H(2)···Cl^-[b]	0.920	0.030
	O–H···Cl^-	0.933	0.027
6···Br^-	C···Br^-	1.249	0.006
	N(1)–H(1)···Br^-[a]	0.999	0.022
	N(2)–H(2)···Br^-[b]	0.949	0.026
	O–H···Br^-	0.933	0.027
6···NO_3^-	C···O^-	1.341	0.003
	N(1)–H(1)···O^-[a]	0.975	0.026
	N(2)–H(2)···O^-[b]	0.947	0.032
	O–H···O^-	0.965	0.038
7···Cl^-	O–H···Cl^-	0.994	0.022
		0.946	0.026
	N(1)–H(1)···Cl^-[a]	0.995	0.022
	N(2)–H(2)···Cl^-[b]	0.961	0.025
7···Br^-	O–H···Br^-	1.010	0.020
		0.966	0.025
	N(1)–H(1)···Br^-[a]	0.094	0.032
	N(2)–H(2)···Br^-[b]	0.095	0.032
7···NO_3^-	C–HO···O^-	1.138	0.007
	N(1)–H(1)···O^-[a]	0.976	0.025
	N(2)–H(2)···O^-[b]	0.950	0.033
	O–H···O^-	0.968	0.038

[a] BCP related to –NH group closer to anthracene ring; [b] BCP related to –NH group closer to benzene ring.